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The Measurement of Carcinogenic Vapors in Ambient Atmospheres

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THE MEASUREMENT OF CARCINOGENIC VAPORS IN AMBIENT ATMOSPHERES

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THE MEASUREMENT OF CARCINOGENIC VAPORS IN AMBIENT ATMOSPHERES

by

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ABSTRACT

Analytical techniques and instrumentation which had been developed during the previous contract years were further evaluated for the collection and analysis of carcinogenic and mutagenic vapors occurring in ambient air. The areas of investigation included: (a) the development of a permeation system for delivering precise quantities of organic vapors for calibration of instrumentation, (b) the development of procedures for the preparation of glass capillary columns for effecting the resolution of complex atmospheric vapor mixtures, (c) the characterization of organic vapor emissions from preset controlled fires, (d) the survey of ambient air samples taken at various sites around the Continental U.S. for the detection of N-nitrosoamines, (e) the identification and quantification of N-nitrosodimethylamines at samples collected in Baltimore, MD and the Kanawha Valley, WV, and (f) the characterization of ambient air for hazardous and background pollutants from several geographical areas within the Continental U.S.

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SECTION 1
INTRODUCTION

This research program on the development of analytical techniques for measuring ambient atmospheric carcinogenic vapors has attempted to furnish a comprehensive and systematic approach to this problem. It has attempted to develop and evaluate the sampling device, field collection methodology, and the entire procedure of the data analysis of carcinogenic vapors in the atmosphere. Until this research program was initiated, the ability to collect and analyze a wide variety of chemical classes from the atmosphere which contained toxic and/or carcinogenic organic compounds was not possible. For this reason, research programs to determine and evaluate the health-impact of carcinogenic compounds in the environment had not been conducted. The ability to execute comprehensive studies on the levels of carcinogenic agents in all media in addition to air and the correlation of this exposure to body burden and health effects on man, was also not possible. Thus, a well-defined epidemiological approach which is required in this type of study, to establish whether an association of relationship existed suffered from the lack of appropriate technology in order to achieve these goals.

The main reasons for identifying and determining environmental carcinogenic organics even at low concentrations are as follows:

(1) A knowledge of the presence and concentrations of mutagens and carcinogen in the air is mandatory for a better understanding of our genetic diseases and the future carcinogenic and mutagenic problems which may arise after a long induction period.

(2) If the incidence of cancer in the US is to be understood and controlled, it will be necessary to determine the concentrations of environmental carcinogens. It is necessary to also understand the complete organic composition of the atmosphere since there are

antagonistic and synergistic relationships i.e. anti-and co-carcinogenic factors which may occur and contribute to the observed incidence of cancer.

(3) It is known that the higher cancer mortality rates have been shown to occur near various sources of air pollution and in statistical studies, it has been demonstrated that cancer associated with the respiratory system is higher where high air pollution occurs.

(4) Because the recent estimates indicate that chemical synthesis adds some 1/4 of a million new chemical compounds each year to the several million already in existance, these new compounds can be a serious source of air pollution and may have a significant affect on the health of the human populace.

and (5) The development of a analytical technique for measuring ambient atmospheric carcinogenic vapors must provide a thorough analytical approach which will measure a wide number of potential environmental carcinogens and mutagens as well as their precursors and various co-factors and anti-factors.

The development of analytical techniques for measuring ambient atmospheric carcinogenic vapors has attempted to provide a conceptual approach which will allow the answering of questions cited above.

SECTION 2
CONCLUSIONS

The design specifications for the cryogenic capillary trap on the inlet-manifold were delineated and evaluated for efficient transfer of vapors from the sampling cartridge to the high resolution gas chromatographic system. The results of this study indicate that a Ni capillary trap of a trans-axial configuration with the dimensions of 0.5 m x 0.04 in i.d. is an optimum design will yield a 100% trapping efficiency for highly volatile vapors such as butane. The compatability of this capillary trap with sample introduction into glass SCOT capillaries without degradation of resolution was also demonstrated.

A permeation system for synthesizing air/organic vapor mixtures for calibration of instruments was designed. The preparation of a series of permeation tubes for calibrating the glc/ms/comp system for analysis of field samples was also achieved. Permeation rates (g/min/cm) ranged from 1×10^{-6} to $\sim 1 \times 10^{-10}$ were achieved using plastic materials (TFE, FEP and polyethylene). The permeation rate was highly dependent on the vapor pressure, the chemical properties of the substance and the plastic material chosen for the preparation of permeation tubes. The use of permeation tubes appears to be a feasible technique for synthsizing accurate and reproducible mixtures of organic/air vapors.

A technique was developed for the preparation of glass capillary SCOT columns. The method increases the reproducibility of preparation of glass SCOT columns while reducing the overall fabrication time to about a 2 day procedure. The preparation of glass SCOT columns utilizes silanized fumed silicon dioxide (6-8 ℓ) suspended in a heavy density solvent (methylene chloride or chloroform) containing the surfactant benzyl triphenylphosphonium chloride and a stationary phase (2-3%). A coating oven was designed and fabricated in order to deposit the stationary phase and finally divided support on the wall of the open tubular column. The coding procedures for

OV-101, DEGS, and Carbowax 20M stationary phases yielded capillaries with HETP values of 0.7-0.9. One hundred meter capillaries can be easily prepared utilizing this technique.

The organic vapors emitted from controlled preset fires were characterized by high resolution glc/ms/comp techniques. The composition of the organic vapors was highly dependent on the stages of burning. The major constituents emitted from the fire during the open flame were benzene (320 ng/ℓ), toluene (891 ng/ℓ), furfural (627 ng/ℓ), p-xylene (529 ng/ℓ) and limonene (622 ng/ℓ). During the open flame period, the major emissions were alkanes, alkenes, and a large distribution of oxygenated compounds (analogs of furan). During the smouldering period, the predominant species were alkanes, and alkyl aromatics. Fewer oxygenated compounds were evident. The major constituents were benzene, toluene and xylene.

The identification and quantitation of N-nitrosodimethylamine (DMN) in ambient air in the Baltimore, MD and Kanawha Valley, WV areas were also conducted. Organic vapors in ambient air on or near an industrial site in Baltimore, MD were collected by adsorption onto a sorbent (Tenax GC 35/60). The pollutants were recovered by thermal desorption and analyzed by gas-liquid chromatography/mass spectrometry/computer using glass SCOT columns. N-nitrosodimethylamine was identified from its mass spectrum as a constituent of the atmosphere by comparison of its mass spectrum with that of authentic DMN. Identical retention times were observed for the unknown and DMN peak on three different capillary columns. N-nitrosodimethylamine levels in ambient air were also determined for an area surrounding this industrial site in Baltimore, MD. Using a Tenax GC cartridge for concentrating DMN and glass capillary gas-liquid chromatography/mass spectrometry with specific ion (m/e 74) monitoring, DMN was quantified. The limit of detection was ~0.3 ppt at 25°C. On the industrial site, DMN levels reached 32,000 ng/m^3 (10.6 ppb) of ambient air. The concentrations of DMN in ambient air collected in the Kanawha Valley were several orders of magnitude lower. The highest values were ~980 ng/m^3 at a location on the plant site in Belle, WV. Many _in situ_ reaction studies were conducted in order to demonstrate whether the formation of DMN on the sampling cartridge could occur in the presence of high concentrations of dimethylamine, NO$_x$ and ozone. Laboratory and field experiments indicated that trace amounts (<30 ppt) of DMN can be formed when very high levels NO_x (>5 ppm), 600 ppb ozone, and 1-5 ppm of amine occur. The concentration of DMN found in the atmosphere was higher than those levels which could be attributed to any type of in situ reaction occurring on the sampling cartridge.

The detection of N-nitrosoamines in samples collected at many different geographical locations within the Continental U.S. was conducted utilizing a computer search of selected m/e ions on previous gc/ms/comp data. Ambient air samples which had been collected over a period of 15 months were subjected to mass fragmentography for N-nitrosodimethylamine, N-nitrosodiethylamine, N-nitrosodi-*n*-butylamine, N-nitrosopiperdine, N-nitrosopyrrolidine, N-nitrosomorpholine, N-nitrosohexylmethylimine, N-nitrosocyclohexylamine, N-nitrosomethylbenzylamine, and N-nitrosophenylamine. Of all these samples which were examined, only those which were taken at the Eisenhower Tunnel in Colorado indicated the presence of N-nitrosodiethyamine (DEN). N-nitrosodimethylamine was tentatively identified. The concentration of DEN was estimated to be ~100 ppt.

The characterization of a number of ambient air samples collected from several geographical areas (Houston, TX and vicinity, Kanawha Valley, WV, St. Louis, MO, Denver, CO, Central and Northern NJ, and Los Angeles, CA Basin) were characterized for hazardous organics. Many halogenated, oxygenated, and nitrogenous organics were detected. The presence of alkanes, alkenes, and alkyl aromatics were ubiquitous in these samples and are probably derived primarily from fossil fuel burning. Several halogenated compounds *e.g.* freon 11, methyl chloride, methylene chloride, chloroform, methylchloroform, trichloroethylene, tetrachloroethylene, monochlorobenzene, dichlorobenzenes, and trichlorobenzenes are present as a general background in all of the samples. The relative amounts however do vary with the sampling site. It is believed that the atmosphere is widely contaminated with low levels of these halogenated compounds. On the otherhand, many halogenated compounds were also detected which were site specific.

The Tenax GC sampling cartridge has proven to be a viable approach for the collection, characterization and quantification of organic vapors occurring in ambient air. The performance of this sampling cartridge has been demonstrated by many studies in geographical areas where a variety of industrial and photochemical types of pollution occur. The technique has performed satisfactorily for the collection of organic vapors under a variety of different meteorological conditions ranging from high to low humidity and temperatures. Some limitations do exist for the highly volatile material such as methyl chloride, methyl bromide, vinyl chloride, vinyl bromide and vinylidine chloride. However, the many other advantages offset the minor disadvantages.

SECTION 3
RECOMMENDATIONS

Six major phases of research should be expanded and pursued: (1) the sampling cartridge should be further examined for potential in situ reactions which might occur during field sampling. This activity should delineate any problems associated with the sampling of atmosphere containing molecular chlorine, bromine or iodine in combination with olefins and NO_x, SO_2 and ozone. Other potential in situ reactions on the sorbent bed should also be examined such as the ozonization of olefins by moderate to high atmospheric concentrations of ozone. (2) The examination of alternate new sorbent materials as a backup or substitute to Tenax GC should be pursued. This may involve the synthesis of analogs or a modified polymer base of Tenax in order to incorporate the desired retention volume properties for organics without increasing the overall background contribution and retention of inorganic gases and water. (3) Further development of capillary technology is recommended. New techniques for the modification of the glass capillary wall to minimize adsorption properties of the semi-polar and polar constituents should be developed. Techniques which circumvent the use of silanization should be pursued. An overall improvement in resolution and column capacity is recommended in order to improve the quantification of complex air mixtures. (4) Extensive sampling of numerous sites for hazardous atmospheric pollutants should be conducted. The methodology for collection, resolution, and identification of hazardous vapors in ambient air which was developed during the past three years under Contract No. 68-02-1228 should be applied to field sampling of numerous sites within the Continental U.S. with a major thrust toward the characterization and identification of carcinogenic and mutagenic vapors. The selection of sites should be based on the high incidence of cancer occurring in these areas, the types of industrial activity or the unique photochemical atmospheric reaction which take place. The selection of sites should include a wide variety of meteorological conditions in order to evaluate the overall techniques. (5) Identification and quantification of hazardous vapors in atmospheric samples should be performed. The identified hazardous vapors should be quantified in ambient air samples and the technique should be evaluated as to its accuracy and reproducibility for monitoring organic vapors in ambient air. And (6) Pollution profiles indicative of individual sites should be developed. Pollution profiles should be assembled for the various geographical areas postulated to contain hazardous vapors. These profiles should indicate site specific pollutants and those vapors which are ubiquitous.

SECTION 4
PROGRAM OBJECTIVES

The general aim of this research program has been to develop and perfect methodology for the reliable and accurate collection and analysis of mutagenic and carcinogenic vapors (hazardous vapors) present in trace quantities in the atmosphere down to ng/m^3 amounts. This information is needed to determine the physiologically active vapors present in polluted atmospheres so that researchers can ascertain their biological impact on populated areas and their overall relationship to the incidence of cancer. The major objectives were:

(1) To further evaluate the inlet-manifold for recoverying organic vapors from sampling cartridges,

(2) The development of a permeation system for synthesizing air/organic vapor mixtures for calibrating instruments which will be used for the quantification of hazardous vapors in the atmosphere.

(3) The development of techniques for the preparation of glass capillary SCOT columns for effecting the resolution of the complex organic pollutants profiles which are observed in ambient air samples.

(4) The characterization of organic vapor emissions from controlled preset fires to ascertain the presence of any hazardous organic vapors.

(5) The identification and quantification of N-nitrosodimethylamine in ambient air by capillary gas-liquid chromatography/mass spectrometry/computer in selected industrial areas suspected to be involved in the production or use of DMN.

(6) The detection of N-nitrosoamines utilizing selected m/e ions and computer search techniques of gc/ms/comp data obtained on ambient air samples over the past fifteen months.

and (7) The identification of hazardous organic vapors in ambient air from several geographical areas in the Continental U.S.

SECTION 5

FURTHER STUDY ON INLET MANIFOLD FOR RECOVERYING ORGANIC VAPORS FROM SAMPLING CARTRIDGES

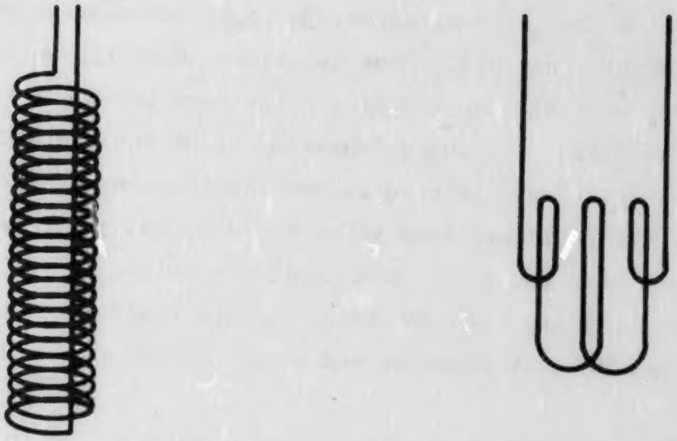
In previous reports,(1-4) we have described an inlet-manifold and had evaluated it in terms of the thermal desorption efficiency of the desorption unit; however, the design specifications for the capillary trap which interfaces the vapors from the sampling cartridge to the chromatographic system had not been thoroughly examined. Some questions about the performance of this capillary trap were (1) the trapping efficiency for a given length and diameter of the capillary, (2) the delineation of whether gold coated Ni capillary or virgin Ni should be used as the fabrication material, (3) the maximum volume of the capillary trap which would be compatible with discrete sample introduction into the glass SCOT capillary column and (4) the configuration of the capillary trap necessary for the cooling and heating cycles in order to ensure efficient trapping and sample introduction into the capillary system.

An experimental evaluation of the capillary trap on the inlet-manifold system was performed and is described in this section.

EXPERIMENTAL

An inlet-manifold system as previously described(1,2,4) was used to evaluate the capillary trap. Capillary traps were constructed of Ni tubing in length of 0.25, 0.5, 1.0, and 1.5 m with an internal diameter of 0.02". Capillary traps were configurated as shown in Figure 1. Two configurations were examined. The first was a co-axial type in which the tubing was wound around the axis of entrance and exit of the purge gas stream and the second was a trans-axial in which the tubing was wound parallel to the entrance and exit of the purge gas.

Gas-liquid chromatography (glc) was conducted on a Perkin Elmer 900 series chromatograph (Perkin Elmer Corp., Norwich, CN) equipped with dual



co-axial

trans-axial

Figure 1. Capillary trap configurations for inlet-manifold.

flame ionization detectors. A 400 ft stainless steel SCOT coated with OV-101 stationary phase was used for resolving synthetic air/vapor mixtures. The column was programmed from ambient temperature to 220°C at 6°/min with an initial and final isothermal periods of 2 and 10 min, respectively. Carrier gas (nitrogen), hydrogen and air flow rates were 6, 30, and 250 ml/min, respectively. The operating parameters for the inlet-manifold were as follows: The thermal desorption chamber temperature was at 270°C, the valve temperature 220°C, and the capillary was cooled to -195°C for trapping vapors and to 180°C for sample introduction into the capillary system. Two purge gas rates were evaluated as to their effect on trapping efficiency (10 and 30 ml/min) during the thermal desorption cycle.

The sampling cartridges loaded with standard air/vapor mixtures contained 1.5 x 6.0 cm of Tenax GC (35/60).

Air/vapor mixtures were loaded onto the Tenax GC sampling cartridges using an exponential decay flask. Known amounts of each organic compound were expanded into a fixed volume and then purged onto the sampling cartridge for capillary trap evaluation.(1,3)

RESULTS AND DISCUSSION

In order to ascertain whether the various trap length and configurations efficiently trapped the organic vapors which were desorbed from the Tenax GC cartridges, the exhaust gas from the capillary trap was routed into a backup Tenax GC cartridge. Using this arrangement, it was determined whether organic vapors had passed through the trap during the cryogenic cooling step. Tenax GC cartridges were loaded with acetone, hexane, benzene, heptane, toluene and chlorobenzene. The Tenax GC cartridges were then desorbed with the vapors passing through the liquid nitrogen cooled capillary traps of co-axial and trans-axial configurations. The backup Tenax GC cartridges were then analyzed by thermal desorption and glc to determine the trapping efficiency of the capillary during the desorption of the front cartridge. By comparison of the quantity of vapors which were trapped in the first step with those which were recovered from the backup Tenax GC cartridge, it was possible to determine the percent trapping efficiency.

The results of this study are summarized in Table 1. The percent trapping efficiency for capillary traps of 1 m and 0.5 m lengths were 100% when the trans-axial trap was 50% submerged into liquid nitrogen. In contrast

Table 1. PERFORMANCE OF CO-AXIAL AND TRANS-AXIAL NICKEL CAPILLARY TRAPS ON INLET-MANIFOLD SYSTEM

Capillary Trap Dimensions	Test Compound	Percent Trapping Efficiency[a]	
		Co-axial Trap	Trans-axial Trap
0.625 o.d. x 0.020 i.d. x 1 m[b]	acetone	90	100
	n-hexane	81	100
	benzene	86	100
	n-heptane	84	100
	toluene	95	100
	chlorobenzene	100	100
0.625 o.d. x 0.020 i.d. x 0.5 m[b]	acetone	89	100
	n-hexane	75	100
	benzene	84	100
	n-heptane	85	100
	toluene	95	100
	chlorobenzene	100	100
0.625 o.d. x 0.020 i.d. x 0.25 m[b]	acetone	84	97
	n-hexane	72	89
	benzene	81	95
	n-heptane	80	96
	toluene	93	99
	chlorobenzene	100	100
0.625 o.d. x 0.020 i.d. x 0.5 m[c]	acetone	-	97
	n-hexane	-	87
	benzene	-	90
	n-heptane	-	98
	toluene	-	99
	chlorobenzene	-	100

(continued)

Table 1 (cont'd)

Capillary Trap Dimensions	Test Compound	Percent Trapping Efficiency[a]	
		Co-axial Trap	Trans-axial Trap
0.625 o.d. x 0.020 i.d. x 0.25 m[c]	acetone	-	74
	n-hexane	-	73
	benzene	-	70
	n-heptane	-	68
	toluene	-	76
	chlorobenzene	-	83
0.625 o.d. x 0.020 i.d. x 0.5 m[d]	acetone	-	0
	n-hexane	-	0
	benzene	-	0
	n-heptane	-	0
	toluene	-	74
	chlorobenzene	-	100

[a] Inlet-manifold conditions were: thermal desorption chamber - 265°C, He purge range - 30 ml/min, valve - 200°C, trap heat - 180°C.

[b] Co-axial and trans-axial traps were completely and 50% submerged, respectively, in liquid N_2.

[c] Trans-axial traps were completely submerged in liquid N_2.

[d] Trans-axial trap was 50% submerged in dry ice/isopropanol coolant.

the percent trapping efficiency varied considerably for the co-axial trap which had been completely submerged in liquid nitrogen (1 m length). The lowest efficiency was observed for n-hexane (81%). For a trap length of 0.5 m, n-hexane vapor was only trapped to an extent of 75%. Non-polar compounds exhibited the lowest trapping efficiency while polar compounds or relatively non-volatile substances exhibited the highest trapping efficiency. In another study, the trans-axial traps were completely submerged. For 0.5 m or 0.25 m traps, the efficiencies were considerably reduced.

The efficiencies of a trans-axial trap cooled to liquid nitrogen and dry ice temperatures were also compared (Table 1). The efficiencies were highest when liquid nitrogen was used. Also when the trans-axial trap was half-submerged the efficiency of trapping was maximum.

A second study was conducted in order to determine whether any decomposition and/or elimination reactions might occur during desorption of organics into the Ni capillary trap or during the heating and injection step onto a gas chromatographic column. To test this possibility, several compounds were selected which were particularly prone to elimination reactions (dehydration or dehydrohalogenation) forming the corresponding olefin. The compounds t-butyl alcohol, 2-bromopentane and cyclohexane iodide were used for this evaluation. These compounds were introduced into the capillary trap via the thermal desorption chamber and cryogenically trapped into the capillary trap followed by heating the trap and injecting the vapor onto the chromatographic column. The corresponding olefin (which might be formed by dehydration or dehydrohalogenation during the cooling and heating cycle of the capillary trap) was monitored on the capillary column. The percent olefin formation and/or parent loss of the compound was determined. The results of this study are shown in Table 2. No dehydration or dehydrohalogenation was observed as either in the loss of parent compound or as the appearance of the corresponding olefin.

In another experiment, decomposition of bis-(chloromethyl)ether (BCME) was studied. BCME was introduced into the capillary trap followed by water since it was known to hydrolyze.(5) As shown in Table 2, the presence or absence of water vapor in the capillary trap during the cooling and heating of BCME did not cause an appreciable loss of the parent compound.

Table 2. CATALYTIC ACTIVITY OF NICKEL CAPILLARY TRAP ON INLET-MANIFOLD SYSTEM[a]

Test Compound[b]	Parent Loss (%)	Product Formed (%)
t-amyl alcohol	0	0
bis-(chloromethyl)ether ($-H_2O$)[c]	0	-
bis-(chloromethyl)ether ($+H_2O$)[c]	0	-
2-bromopentane	0	olefin (0)
cyclohexane iodide	0	cyclohexene (0)

[a] Inlet-manifold parameters were: thermal desorption chamber - 265°C, He purge rate - 30 ml/min, valve - 200°C, trap cooling cycle - -195°C, trap heating cycle - +180°C.

[b] Approximately 1 μg of each compound (except BCME) was tested for decomposition.

[c] Approximately 200 ng of BCME was tested, 1 mg H_2O was added to trap.

Gold coated Ni capillary traps did not exhibit better performance characteristics using these experimental tests.

One of the problems that was evident in the use of a capillary trap with an internal diameter of 0.02" was the freezing of the trap during the introduction of vapors from a sampling cartridge which contained a relatively high amount of water vapor as a result of sampling in areas with high humidity. The problem of obstruction of purge gas flow through the trap was enhanced when the trans-axial trap was 50% submerged in liquid nitrogen. In separate experiments, the use of a larger diameter capillary (0.04") was examined. The trapping efficiencies were repeated using lengths of 0.25, 0.5 and 0.75 m with an internal diameter of 0.04". The trapping efficiency for the trans-axial remained unchanged when purge rates of 10 or 30 ml/min were used. High humidity sampling was conducted (90%, 90°F) and thermal desorption analysis was conducted utilizing these traps. Obstruction of gas flow or complete plugging was not observed in these cases. However it was found that a minimum trap length of 0.5 m was still necessary in order to efficiently recover all the vapors desorbed from the Tenax GC sampling

0.5 m length trap with a 0.04" diameter provided quantitative recoveries of thermally desorbed vapors for thermal desorption periods of upto 15 min.

The use of 0.5 m x 0.04" i.d. capillary traps was also examined for compatibility with the glass SCOT columns. Particular attention was addressed to the problem of band (peak) spreading which occurs when excessive dead volume is present in sample introduction mode. Experiments utilizing 400 ft stainless steel SCOT capillaries, or 100 m glass SCOT capillaries coated with OV-101 indicated that no band spreading occurred when the larger i.d. trap was employed. The possibility of using this inlet-manifold system with wall coated open tubular (WCOT) columns remains to be demonstrated since the low dead volume requirements for these capillaries are more stringent than for SCOT capillaries.

SECTION 6

PERMEATION SYSTEM FOR SYNTHESIZING AIR/ORGANIC VAPOR MIXTURE FOR CALIBRATING INSTRUMENTS

There are four general factors which affect the sensitivity of an analytical procedure for analysis of carcinogenic vapors in ambient air. These are: (1) efficiency of the sorbent medium in trapping organic vapors, (2) the efficiency of the thermal desorption manifold in delivering collected samples to the column, (3) the efficiency of the chromatographic column in transmitting the desorbed vapors through the glass capillary and (4) the response of the mass spectrometer. Calibration for quantitative analysis must systematically account for all of these factors. The response of the glc-ms system to known quantities of specific compounds may be observed; however, this does not take into account systematic errors in sample collection. It is also difficult to deliver aliquots of concentrations (ppt) near the lower detection limits so that calibration plots need to be extrapolated out of their region of validity. Long term variation in sensitivity of the analytical system could occur as well. To overcome this numerous compounds could be used for calibration. Sensitivities of vapor relative to standard compounds in the glc-ms system may be measured. Aliquots used as standards may be added to samples before analysis. Errors in desorbing and transfering vapors to the analytical system are circumvented.

Sampling of air doped with known trace quantities of vapors would account for errors inherent in collection and analysis procedures, but such low concentrations are subject to rapid depletion by adsorption onto surfaces of vessels used for providing calibration standards. This problem could be circumvented by the use of permeation tubes which at constant temperature emit vapor at a constant low rate. A stream of air or nitrogen passing over a group of permeation tubes in a thermostated chamber would pick up a low concentration of vapor from each tube. Surfaces in the flow system should become equilibrated with these compounds so that they would be delivered from the system at the same rate that they were emitted by the permeation tubes.

The permeation rate can be determined gravimetrically by weighing each tube at periodic intervals.

A stream of nitrogen passing over a permeation tube could be used to deliver a minute quantity (10^{-7}-10^{-9} g) of a typical pollutant vapor or a standard compound to a cartridge. It also could be used to deliver very small concentrations of vapor into a stream of air in order to imitate the conditions which are obtained during sampling of polluted air. Use of permeation tubes for calibration of instruments (e.g., glc-ms) should effectively minimize systematic errors.

A flow system for the purpose of calibrating a glc-ms-comp system using permeation tubes was designed and fabricated. Experiments have been conducted to determine the most suitable materials for use as permeation tubes and this section discusses these results.

EXPERIMENTAL

The designed flow system is depicted in Figure 2. The components were connected with 1/8" o.d. stainless steel tubing. The Pyrex permeation chamber (25 mm i.d. x 44 cm in length) was enclosed in a jacket through which an ethanol-water mixture was circulated from a constant temperature bath (Haake Model FE circulating pump and thermostated heater coupled with Haake Model C11 refrigeration unit). Before entering the permeation chamber, the nitrogen was passed through a temperature equilibration coil which was approximately 4 mm i.d. x 1 m in length. Upon leaving the chamber, the nitrogen vapor stream passed through a 100 ml mixing chamber before being split. A flame ionization detector (Varian Model 1440, Walnut Creek, CA) served to demonstrate whether the rate of sample delivery was constant as well as providing a means for discarding a constant fraction of sample. A pair of rotometers (Brooks Instrument Div., Emerson Electric Co., Hatfield, PA, Type 1355, tube size R-2-15-AAA with glass float) were installed in each branch of the flow system. A reproducibility of ± 0.5 ml/min was observed throughout its operating range for the rotometer which measured flow through the cartridge. Reproducibility for the rotometer which was upstream of the flame ionization detector was poor at flow rates >35 ml/min, due to the flow resistance of the flame ionization detector and attached fittings. With the flame ionization detector removed from the system, reproducibility for this rotometer was also ± 0.5 ml/min throughout its operating range (Fig. 3). A large

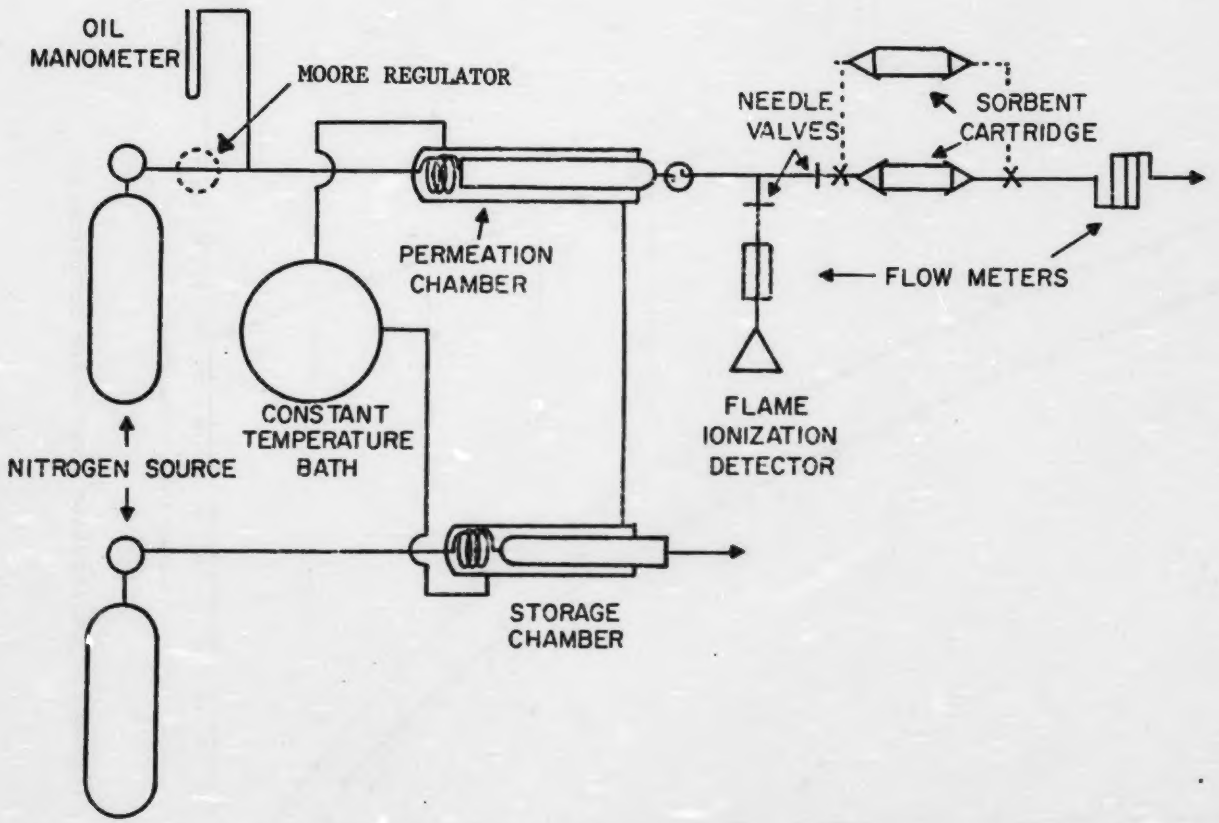

OIL MANOMETER
MOORE REGULATOR
NEEDLE VALVES
SORBENT CARTRIDGE
PERMEATION CHAMBER
FLOW METERS
CONSTANT TEMPERATURE BATH
FLAME IONIZATION DETECTOR
NITROGEN SOURCE
STORAGE CHAMBER

Figure 2. Permeation system for delivering constant concentrations of organic vapors.

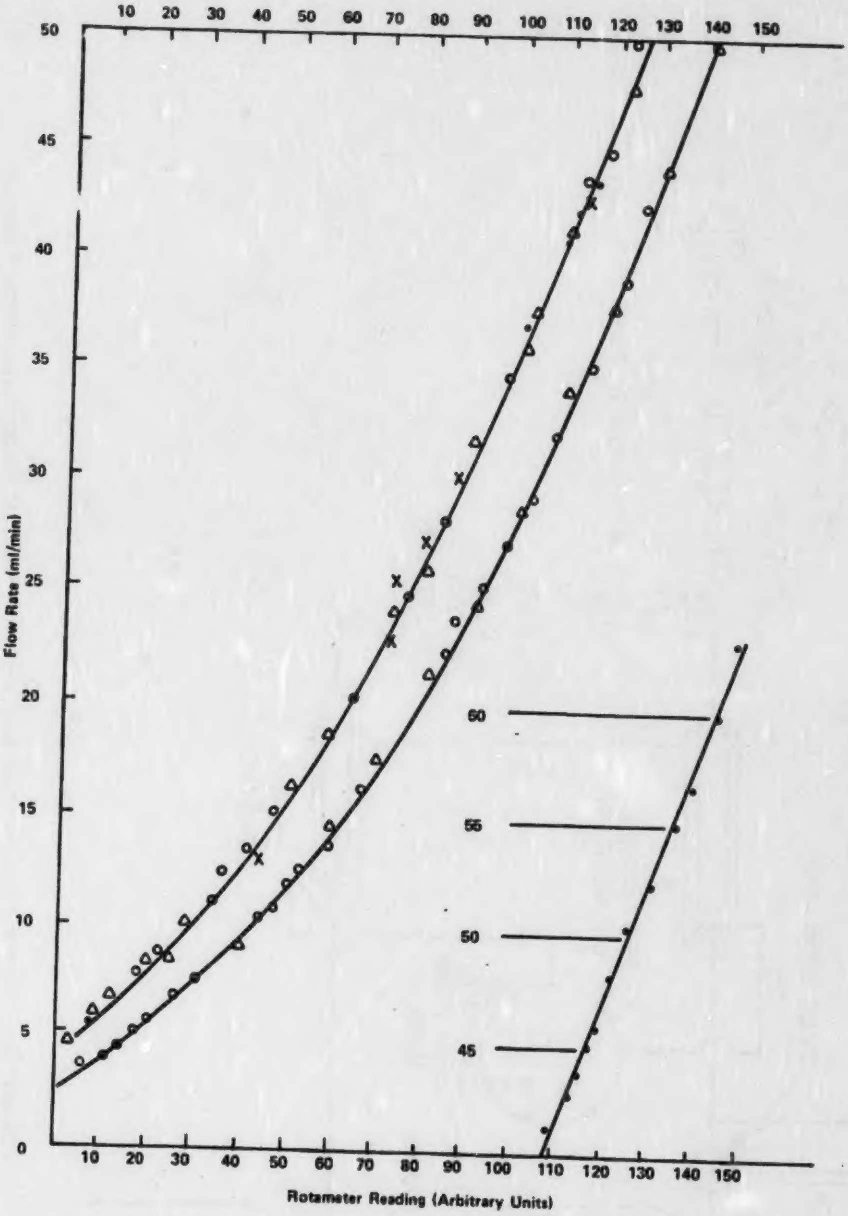


Figure 3. Calibration curves for rotometers.

permeation chamber connected to the constant temperature bath and flushed continuously by a 100 ml/min nitrogen stream was used to store permeation tubes. This permitted calibration of the tubes without interfering with operation of the flow system and immediate use of stored tubes without waiting for equilibration of the permeation rate.

This system could be used either to load sorbent cartridges (Fig. 2) or to deliver vapors to a stream of air entering a cartridge sampler (Nutech Model 221, Durham, NC). The cartridge holder consisted of two Beckman Teflon® reducing unions (No. 830511) for holding sampling cartridges. The upstream union was fitted with Teflon® plug which had a 2 mm i.d. bore to minimize dead volume.

In order to access the range of permeation rates which might be encountered among organic vapors of varying polarity, permeation tubes for several typical compounds were prepared. They were made of approximately 7-15 cm lengths of plastic tubing. Four kinds of tubing were used. Surgical grade polyethylene tubing of 0.082 in o.d. x 0.062 in i.d. was initially used, but it gave permeation rates for most compounds which were too high compared with the volume of the tube. Subsequently 0.25 in o.d. x 0.19 in i.d. tubing made of polyethylene (PE), and two types of Teflon®, tetrafluoroethylene (TFE) and fluorinated ethylene and propylene (FEP), were used. The ends were closed with glass plugs secured by stainless steel ferrules. This technique was used with dimethylamine which has a vapor pressure well above one atmosphere at ambient temperatures. The plastic tubing and the end plugs withstood the pressure, but the permeation rate from the polyethylene tube (7 x 10^{-5} g/min) was too large to be useful. Many non-polar compounds of much lower volatility also had extremely high permeation rates from polyethylene tubes.

RESULTS AND DISCUSSION

Performance of Permeation Tubes

Permeation rates obtained for typical organic compounds at 25°C are shown in Table 3. The tubes were weighed on a microbalance at intervals of about one week. The plots of weights (grams) vs time (min) were linear (Fig. 4). Permeation rates were determined from such data by two methods: (1) by dividing the weight loss (g) by the time interval (min) and (2) by applying

Table 3. APPROXIMATE PERMEATION RATES OF AMBIENT AIR POLLUTANTS FROM PLASTIC MATERIALS

Compound	Permeation Rate[a] (g/min/cm)	Material[b]
methylene chloride	1.37×10^{-6}	TFE
methylene chloride	2.83×10^{-8}	FEP
chloroform	8.15×10^{-7}	TFE
chloroform	4.07×10^{-9}	FEP
carbon tetrachloride	8.57×10^{-10}	TFE
carbon tetrachloride	6.53×10^{-10}	FEP
phenylacetylene	4.09×10^{-9}	TFE
phenylacetylene	4.17×10^{-9}	FEP
toluene	7.70×10^{-9}	TFE
toluene	6.87×10^{-9}	FEP
m-dichlorobenzene	7.11×10^{-8}	TFE
m-dichlorobenzene	1.21×10^{-8}	FEP
1,1,1-trichloroethane	2.57×10^{-9}	TFE
1,1,1-trichloroethane	2.27×10^{-9}	FEP
acetonitrile	2.5×10^{-7}	PE
acetone	2.5×10^{-8}	PE
acetone	1.6×10^{-8}	TFE
acetone	3.1×10^{-9}	FEP
benzene	8.3×10^{-6}	PE
benzene	8.4×10^{-9}	TFE
benzene	5.0×10^{-9}	FEP
2-propanol	5.7×10^{-8}	PE
dimethylamine	6.9×10^{-8}	TFE
dimethylamine	8.0×10^{-9}	FEP
trichloroethylene	1.1×10^{-7}	TFE

[a] Rates were obtained for 25°C.

[b] PE = surgical grade polyethylene tubing (0.082 in o.d. x 0.062 in i.d.), TFE and FEP = Teflons® (0.25 in o.d. x 0.188 in i.d.)

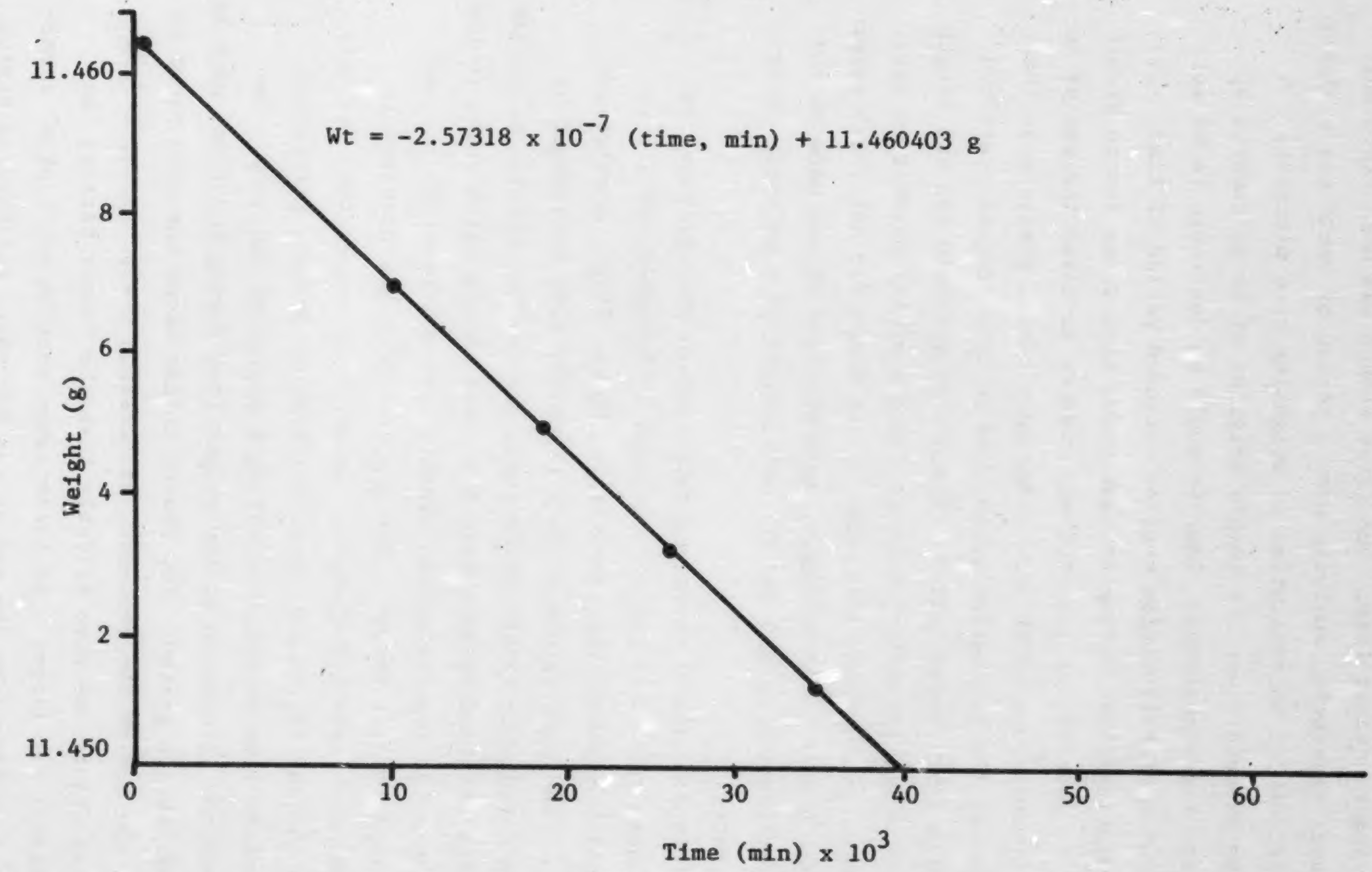


Figure 4. Permeation rate for benzene in TFE Teflon® at 20.0°C. Tube dimensions were 0.25 in o.d. x 0.188 in i.d. x 12.5 cm in length.

linear regression analysis to the plot of weight vs time to obtain the negative slope of the least squares line. The first method was more rapid but less precise. Linear regression analysis over a period of weeks was a slower process, but the effects of uncertainties in weighting were minimized. A disadvantage of the procedure was the weekly weighing of large numbers of tubes which was very time-consuming. Thus it would be desirable to be able to rely on the results of calibration over an extended period of time. The literature on permeation tubes indicates that permeation rates remain stable for a long time.(6) However the reported experiences involved the use of inorganic or light hydrocarbons which were under substantial pressure in the plastic tube. Most of the permeation tubes used in this program contained organic liquids with lower volatilities. Another uncertainty was the length of time required by a new permeation tube to reach a stable permeation rate. During calibration it was evident that some of the tubes did not reach stable rates for more than a month. Accordingly, an investigation was made of the length of the stabilization period and the reliability of previously determined permeation rates.

Several additional organic vapor permeation tubes were prepared in January, 1976. These tubes and the one prepared in November, 1975 were gravimetrically calibration during February and March, 1976. Results are shown in Table 4. The first column of data gives the rate determined by linear regression during the months of February and March. The second column depicts the results obtained by extending the least square calculation to the end of April. Where the results agreed closely, permeation rates had been steady over the experimental period. For many of the tubes prepared in January, the permeation rate had changed. In order to see whether the rate had stablized by the end of the Feb.-Mar. calibration period, permeation rates were determined from weight loss during a period of one week. The third column shows the rate based on the weight loss during the final week of the Feb.-Mar. calibration period. The fourth column shows the rate based on weight lost from the end of the Feb.-Mar. calibration period to the end of April. The latter figure was more reliable than the former because the experimental interval was larger. If these rates were in substantial agreement, the rate had stablized by the end of the Feb.-Mar. calibration period. In many cases the rate had not stablized, and a new calibration period was

Table 4. RATE OF WEIGHT LOSS FOR PERMEATION TUBES DETERMINED OVER AN EXTENDED PERIOD OF TIME

			Permeation Rate By Linear Regression		g/min by Interval Weight Loss	
Date Started	Compound	Plastic	Feb.-Mar.	Extended to April	Feb.-Mar. (1 week)	April
11-75	acetone	PE	1.75	1.74	1.77	1.74×10^{-6}
11-75		TFE	4.15	3.97	4.05	3.96×10^{-7}
11-75	benzene	FEP	6.00	4.87	5.64	5.90×10^{-8}
11-75	benzene	TFE	2.48	2.44	2.47	2.42×10^{-7}
11-75		FEP	2.43	2.47	2.70	2.47×10^{-8}
1-76	benzene-d_6	TFE	1.03	1.64	1.52	1.70×10^{-7}
1-76		FEP	24.6	9.48	16.7	7.54×10^{-8}
1-76	dichloromethane	TFE	6.43	2.28	2.52	2.06×10^{-6}
11-75		FEP	3.02	3.01	3.03	2.99×10^{-7}
1-76	chloroform	TFE	1.14	1.14	1.15	1.14×10^{-6}
11-75		FEP	2.43	2.47	2.70	2.47×10^{-8}
1-76	toluene	TFE	0.617	1.07	0.886	1.15×10^{-7}
1-76		FEP	4.49	4.07	3.04	4.09×10^{-8}
1-76	phenylacetylene	TFE	2.76	4.12	3.78	4.28×10^{-8}
1-76		FEP	23.0	9.54	12.4	8.21×10^{-9}
1-76	1,1,1-trichloroethane	TFE	13.8	8.75	10.8	8.63×10^{-8}
1-76		FEP	7.19	2.03	1.18	2.18×10^{-9}
1-76	tetrachloroethylene	TFE	0.248	1.50	0.568	1.61×10^{-7}
1-76		FEP	11.6	6.52	9.50	6.16×10^{-8}

(continued)

Table 4 (cont'd)

			Permeation Rate By Linear Regression		g/min by Interval Weight Loss	
Date Started	Compound	Plastic	Feb.-Mar.	Extended to April	Feb.-Mar. (1 week)	April
1-76	chlorobenzene	TFE	0.823	1.07	0.892	1.10×10^{-7}
1-76		FEP	2.78	1.31	1.68	1.18×10^{-6}
1-76	m-dichlorobenzene	TFE	3.75	3.40	2.74	3.45×10^{-7}
1-76		FEP	5.56	2.57	3.68	2.29×10^{-8}
1-76	methyl ethyl ketone	PE	1.94	1.90	1.94	1.83×10^{-6}
1-76	ethyl acetate	PE	3.75	3.60	3.71	3.59×10^{-6}

initiated to determine the eventual permeation rates that was attained. Those tubes which had reached a stable permeation rate were to be subjected to an additional test. They have been placed in cold storage. After two weeks, they will be returned to storage in a thermostatic chamber at 20°C and their ability to return quickly to their former permeation rate will be assessed. These results will be presented in the next annual report.

The carbon tetrachloride tubes did not perform as reliably as the other permeation tubes. The TFE and FEP tubes never reached a sustained permeation rate above 10^{-9} g/min. During some intervals they actually gained weight. It was thought that this might have been caused by storage of dimethylamine tubes in the same chamber, but the effects were later observed to be apparently independent of the presence of dimethylamine tubes. The polyethylene tube, on the otherhand was stablized within two weeks, but permeated at a very high rate and was depleted in a short period of time.

In summary, organic vapor permeation tubes may require two months or more to reach a steady permeation rate (particularly for $<10^{-7}$ g/min rates).

Performance of Permeation System

A study was conducted to determine whether background contamination was occurring either from the nitrogen carrier gas in the flow system or from the emission of vapors by the plastic tubing. Empty 10 cm lengths of polyethylene TFE and FEP tubing were placed in the permeation chamber, and sampling with Tenax cartridges was conducted for a period of 3 hrs with gas passing through the system. Tenax GC cartridges were then desorbed and analyzed by glc-fid. No evidence of background from these plastic materials was observed.

In order to demonstrate the feasibility of the fabricated permeation flow system, pilot experiments were conducted to test its ability to measure and deliver aliquots of vapors to sampling cartridges. This ability depended upon two assumptions: (1) that the delivery rate was a function of the permeation rate from the tube and not on the flow rate of the carrier gas (the flow rate being much larger than the permeation rate and constant) and (2) that the carrier gas flow was split proportionately to the flow of entrained vapors. The validity of these two assumptions was examined for the flow system and the effects of variations in pressure in the permeation chamber and variations in room temperature were also investigated.

During the operation of the system with the splitting of flow, a sinusoidal signal from the flame ionization detector was observed. When most of the flow was directed to the flame ionization detector, this variation never exceeded ±4% of the total signal, but when only a small fraction of the flow passed through the FID, the variation approached ±20%. Thus the variation appeared to be pressure dependent. An oil monometer was placed upstream from the permeation chamber (Santovac-5 diffusion pump oil, 1.18 g/ml, 1 cm = 0.846 torr = 0 017 psi). In this manner it was discovered that the sinusoidal variation in the flame ionization detector tracing could be minimized by maintaining the system at a pressure substantially below 10 cm of oil. The problem apparently resulted from a variation in the downstream pressure of the nitrogen regulator, a common problem with such regulators.

The effect of pressure on the performance of the system was also investigated. With all of the flow directed to the flame ionization detector, the 20 turn needle valve (Hoke 1335G2Y) was abruptly closed two turns from half opened position. There was a momentary deflection ~30 sec in the FID trace, at which time it returned to its previous level, as did the rotometer float. The oil mometer indicated a slight increase in pressure. When this process was repeated until a pressure above 10 cm oil was reached, the flow rate decreased and the flame ionization detector signal surged, then decreased and become constant.

It was believed that the room temperature might also effect the flow system by causing variations in the amount of material adsorbed on the walls of the non-thermostated connecting tubing. Daily variations of room temperature as large as 13°C were observed and a continuous variation over a 2°C range was normal. To test the possibility of adsorption/desorption a heat gun was used to heat a section of the tubing leading to the flame ionization detector. Although this would represent a more drastic variation than was normally observed in the ambient temperature, the response of the flame ionization detector to this was negligible.

The assumption (No. 1) that the rate of the delivery of vapors was dependent on the permeation rate was tested by delivering a stream of nitrogen which had passed over a benzene permeation tube (2.57 x 10^{-7} g/min at 20°C) to 5 cartridges (one at a time for 5 min) at a rate of 49 ml/min. The flow rate was then changed to 32.5 ml/min and after equilibration of the system 3 more cartridges (5 min per) were loaded. All the cartridges were then thermally desorbed and analyzed by gc with flame ionization detector (a 200 ft OV-101 SCOT capillary was used on a Perkin-Elmer 900 programmed from 30-120° @ 4°/min). The peak areas were measured with a planimeter. The results indicated that there was no significant change in the rate of benzene delivered to the cartridges due to a 34% decrease in the flow rate, provided that time was allowed for the concentration of vapor in the carrier gas to equilibrate. Such variation as was observed in the peak areas was probably due to continued small variations in the flow rate and to the uncertainty (±5%) in the 5 min collection period.

When the flow was split ~1:1 between the cartridge and the flame ionization detector, some inbalancing of the flow rate upon insertion of the cartridge was observed. This was probably due to an additional contribution to flow resistance as offered by the cartridge. Somewhat smaller peaks than would have been anticipated from the benzene permeation tube were observed.

The ability of the flow system to deliver aliquots of vapors to sampling cartridges was further tested by using it to calibrate a gas chromatograph with flame ionization detection and a glc-ms-comp system. For the purpose of calibrating a gc-fid system, dichloromethane, chloroform, benzene and toluene were selected. Benzene and dichloromethane were used to calibrate the glc-ms system.

Permeation tubes containing dichloromethane, chloroform, benzene and toluene were placed together in the permeation chamber (Fig. 2). Nitrogen carrier gas at a flow of ~6 ml/min was passed over the permeation tubes and the effluent stream split. One portion of this stream was exhausted into a fume hood and the other portion was passed through a Tenax cartridge.

Sampling cartridges were loaded with calculated amounts of each of the vapors. The permeation rate and the loading time was related by the following expression:

$$G_a = \frac{F}{F + B} \cdot P_a \cdot t$$

where G_a = g of vapors a loaded on cartridge
F = ml/min of flow to cartridge
B = ml/min flow by-passed
P_a = permeation rate for vapor a (g/min)
t = loading time

After the cartridges were loaded with known amounts of vapors, they were thermally desorbed and analyzed by gc-fid (Perkin-Elmer Series 900 gas chromatograph equipped with a 200 ft OV-101 SCOT capillary). Peak areas for each of the constituents were measured with a planimeter and a linear regression analysis of the data was performed. The linear regressions are shown in Figure 5. Also included are the 95% prediction intervals, which indicate that 1 out of 20 analyses would fall outside of this range.

Calibration of the glc-ms system was also performed for benzene and dichloromethane. Single ion monitoring was used in both cases (benzene-m/e 78, dichloromethane-m/e 49); however, in this case each compound was individually examined. The calibration plots with the 95% prediction intervals are shown in Figure 6.

The large prediction intervals indicated that improvements in the precision of the method were required. There were two evident sources of uncertainty which could be minimized: (1) the fluctuation in the flow rate and the split ratio during loading of cartridges, (2) inaccurate measurements of the time of loading because of the complicated procedure of replacing an empty tube with a cartridge and fitting the connection to the sampling cartridge.

Three modifications to the system were made in order to improve its precision: (1) The flow rate and pressure of nitrogen carrier gas to the system was stablized. Use of ordinary nitrogen pressure regulator with a needle valve to regulate the gas flow was inadequate. The flow was not constant but varied sinusoiduly and this effect was multiplied by the method used to split the gas stream. Stabilization of the flow delivered to the system was achieved using a Moore regulator placed in line immediately upstream of the permeation chamber. This permitted rapid equilibration of chamber pressure and afforded a maximum resistance to changes in pressure caused by changes in the split ratio or the flow rate through the chamber. (2) The oil monometer was replaced. The high viscosity of the oil precluded rapid response to changes in line pressure. This often led to operation of

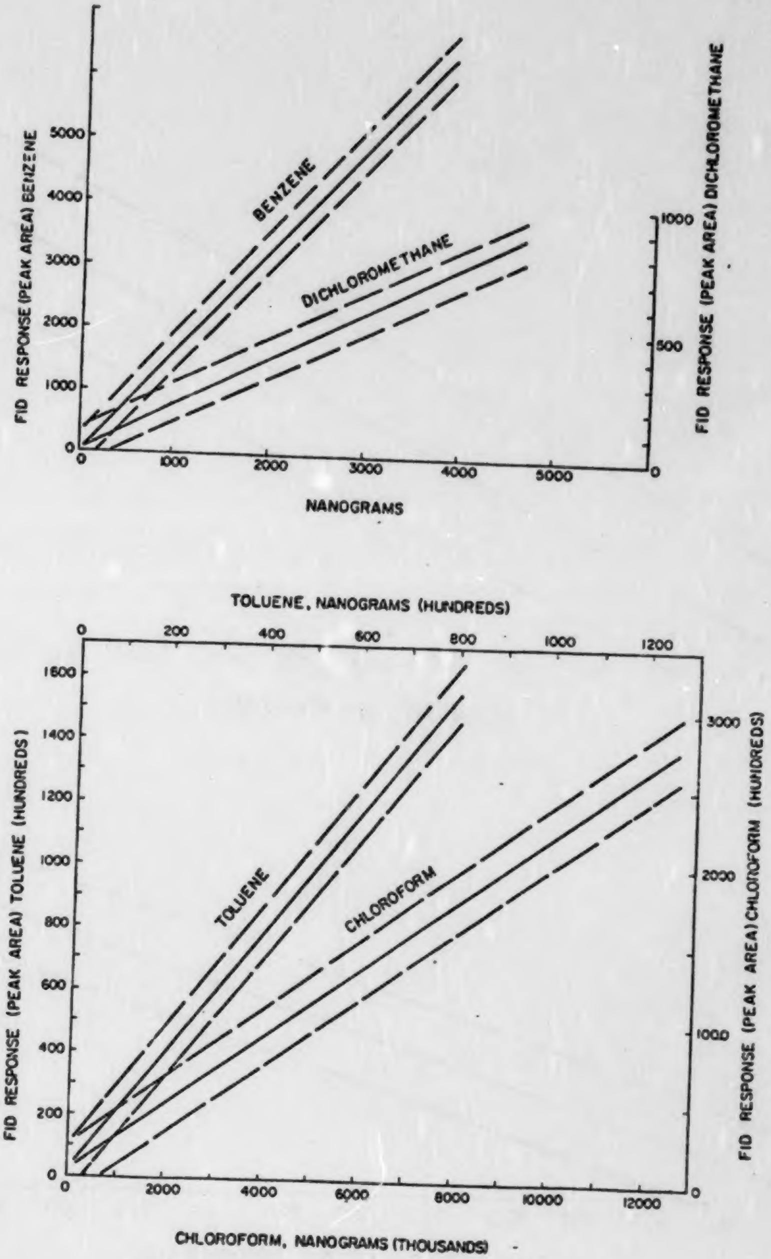
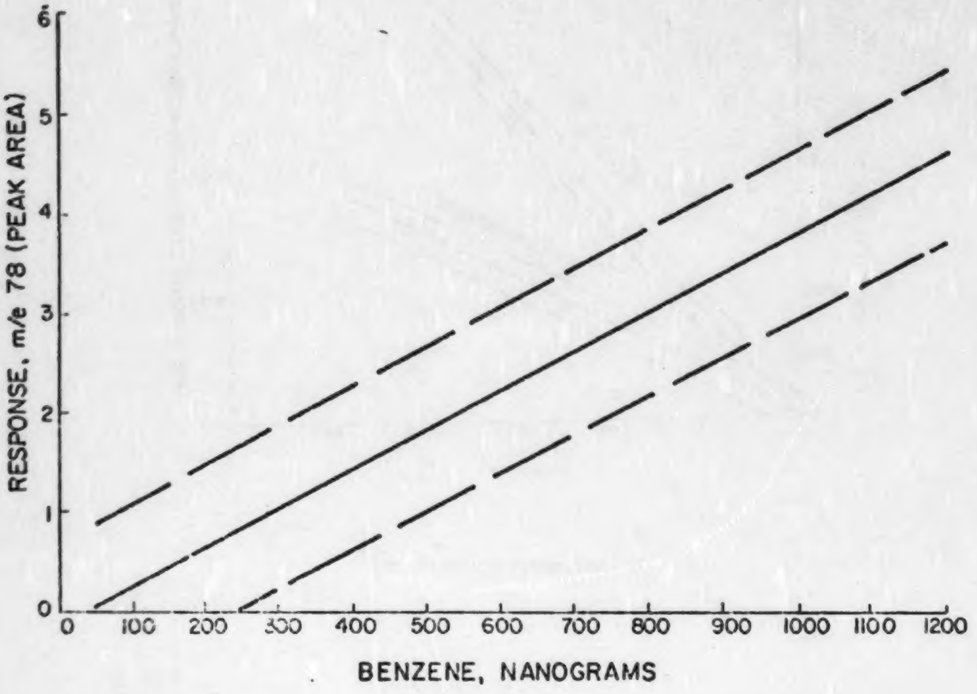


Figure 5. Linear regression of flame ionization response *vs*. weight of substance.



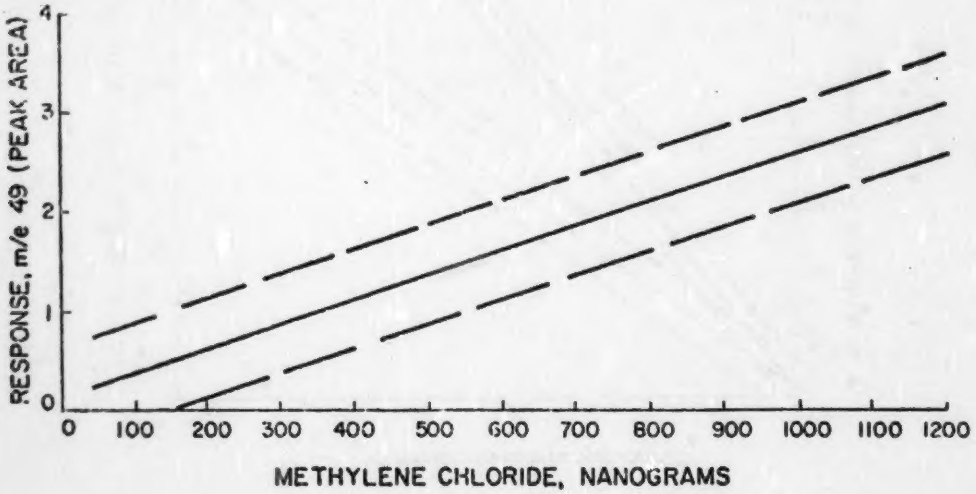


Figure 6. Linear regression of mass spectrometer response (single ion mode) vs. weight of compound.

the system under conditions of changing pressure (and therefore flow rate). The monometer was replaced with a Matheson 63-3101 pressure gauge having a range of 0-15 in water. (3) The process of introducing and removing cartridges resulted in an uncertainty in the sampling time of about 20 sec. To obtain acceptable precision longer sampling times were required. Reduction in the uncertainty of the sample collection period was accomplished by installing a by-pass (dashed lines in Fig. 2) to permit the flow to be maintained while the cartridge is inserted. Reduction of the time variation by a factor of about 10 was achieved. Teflon plug three-way stopcocks were used. They were observed to operate without leaking at the pressures prevailing in the system.

The precision of the system could be further improved by installing a flow controller in place of the needle valve used to direct carrier gas to the cartridges. In the present system small variations in flow resistance of individual cartridges result in slight alterations in the split ratio. This effect is not a serious source of error but its elimination could effect a further increase in precision.

SECTION 7

DEVELOPMENT OF TECHNIQUE FOR THE PREPARATION OF GLASS CAPILLARY SCOT COLUMNS

Glass open tubular columns have several advantages. They have superior resolving power, generally require lower operating temperatures, are much less apt to catalyze rearrangements and/or degradation of reactive substances and can be demonstrated to pass compounds that normally would fail to be transmitted through metal open tubular capillary columns.(7) There are a number of methods in the literature which have been reported for coating capillaries which implies that the coating technique has remained a major problem area. Most of the methods that have been suggested fall into two general categories: (1) those which utilize a dynamic method in which a relatively concentrated (~10%) solution of liquid phase and an appropriate solvent is passed through the column under highly controlled flow conditions,(7) and (2) a static technique in which the column is completely filled with a relatively dilute (~1%) solution of the liquid phase and as the solvent is evaporated under vacuum and the residual phases deposited hopefully as a thin uniform film on the inner column wall.(7)

A new method has been developed for preparing glass open tubular columns which allows the preparation of capillaries in a very routine and simple manner. The procedures that have been developed are described here and are based upon the modification of the procedures reported by Jennings, *et al.*,(8) German, *et al.*,(9,10) and Pellizzari.(11)

EXPERIMENTAL

A Hupe-Busch glass drawing machine (Hupe-Busch Karlsurhe Germany) was used for preparing capillaries of various diameters and lengths.

Prior to drawing the glass capillary, the tubing (8 mm o.d., 4 mm i.d., and 2 m in length) was washed with acetone, methanol, methylene chloride and dried. Prior to drawing short pieces (6-8 in) of tube are attached in order to increase the effective drawing length. Lengths of up to 130 m can be drawn for capillaries which have an internal diameter of 0.30 mm.

After drawing the capillary, the capillary was washed with 50 ml of acetone and methanol. Glass capillaries were silanized with a 10% solution of dimethyldichlorosilane and toluene followed by rinsing with toluene, methanol and acetone using ~20-30 ml of each solvent. The coating solution consisted of 0.1% surfactant (benzyl triphenylphosphonium chloride), 0.1% of Silanox® and 2.0-3.5% of stationary phase in methylene chloride. Prior to filling the capillary with the coating solution, a 1-2 ml quantity of methylene chloride was introduced as a wetting plug in front of the coating solution. The coating solution was forced into the capillary using a pressurized reservoir. The glass capillary was entirely filled with the coating solution and one end sealed with a flame.

A coating oven(8) was fabricated as shown in Figure 7. The column was placed on the drive shaft of the oven and the spring-loaded drive-follower was positioned. Two coils of the open end of the filled column was rotated into the oven. Then the oven temperature was raised to 150°C and the inlet-coil tube which passes the capillary through the oven wall was heated to 200°C. The drive motor was then energized at a rate of 13 revolutions/minute. The drive shaft on the apparatus had a diameter of ~12.7 mm. A period of ~1.5 hr was required to drive a 100 m capillary into the coating oven. All but the last two coils of the capillary was driven into the oven and then the sealed end was broken. Through the capillary helium gas was passed at a rate of ~4-6 ml/min for a period of 30 min. This step was necessary to remove all residual solvent prior to cooling the capillary. The oven was then cooled and the capillary removed. The first and last five coils of the capillary were discarded and the column was then ready for use.

RESULTS AND DISCUSSION

During the developmental stages, some difficulty was encountered in the drying step of the coating procedure. The deposition of the Silanox® which served as a support material was often uneven. The position of the vapor liquid interface did not always remain constant and some bumping occurred. Adjustment of the percent of Silanox® to 0.1% yielded a more evenly coated capillary. Perhaps the use of higher density solvent such as Freon 113 which has a boiling point similar to methylene chloride but a density between chloroform and carbon tetrachloride would be more appropriate as a medium for suspending the Silanox®. The density provided by Freon 113 may

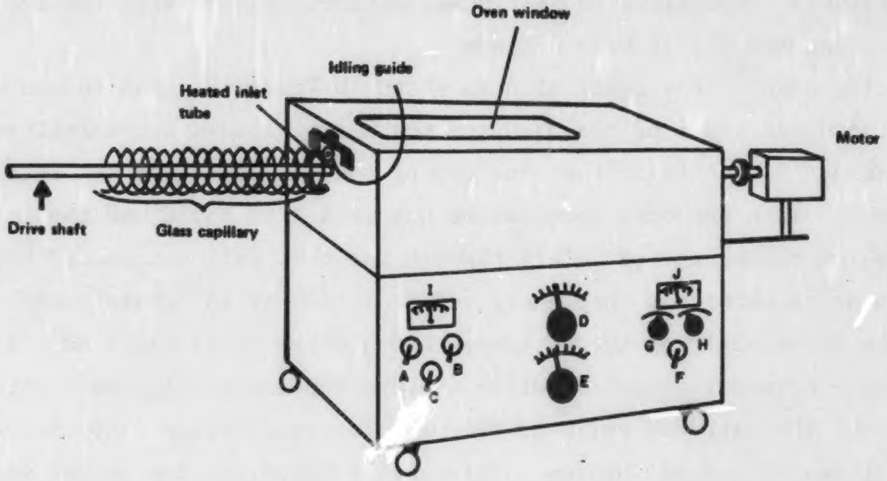

Oven window
Idling guide
Heated inlet tube
Motor
Drive shaft
Glass capillary
I
J
A
B
C
D
E
F
G
H

Figure 7. Glass capillary coating oven.

ensure that the precipitation of the silanized fumed silicon dioxide (6-8 μ) would not occur and a more uniform deposition of the support could be achieved on the inner capillary wall.

The mechanism for deposition of the silanized fume silicon dioxide and liquid phase occurs during the introduction of the filled capillary into the heated inlet zone of the coating oven where an aerosol is formed which disperses the liquid phase and Silanox® onto the wall. Under these conditions any liquid phase can be forced to coat the column, however whether it remains as a thin coherent film probably depends upon the degree of attraction between the glass surface and the liquid phase as opposed to the cohesive forces or surface tension of the liquid phase.

The procedures described here were used for preparing OV-101, OV-225, DEGS, and Carbowax 20M stationary phase coated SCOT columns. The highest success was observed for OV-101 and Carbowax 20M as judged from the observed number of theoretical plates.

A comparison of a 42 m glass SCOT capillary prepared as described above and a commercial 400 ft stainless steel SCOT capillary also coated with OV-101 are shown in Figures 8 and 9, respectively. A duplicate set of Tenax GC sampling cartridges which contained ambient air sampled in C. H. Milby Park in Houston, TX was used for this evaluation. A higher intensity of lower eluting materials was observed in the glass capillary than for the stainless steel column. This implies that the percent transmission of the pollutants from ambient air was better for the glass capillary column. Another example is given in Figure 10.

Longer glass capillary columns need to be investigated for comparison with the stainless steel SCOT capillaries. Various combinations of coating solutions (semi-polar and polar) also need to be examined for the preparation of capillaries which will resolve ambient air pollutants of interest using the new developed procedure.

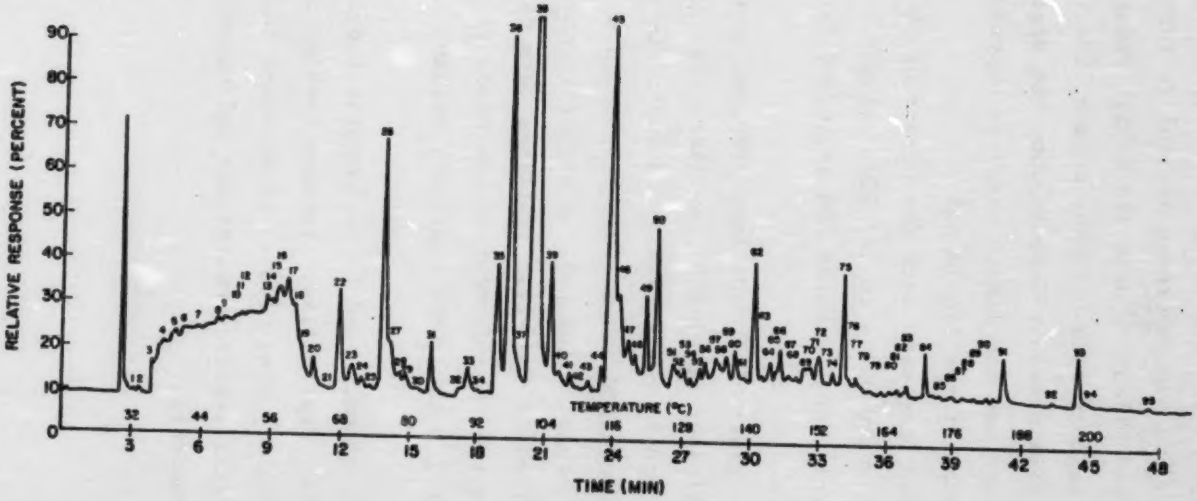


Figure 8. Profile of ambient air pollutants obtained for C. H. Milby Park, Pasadena, TX using glass capillary gas chromatography/mass spectrometry/computer. A 42 m glass SCOT coated with OV-101 stationary phase was used; temperature programmed from 20-220°C @ 4°C/min.

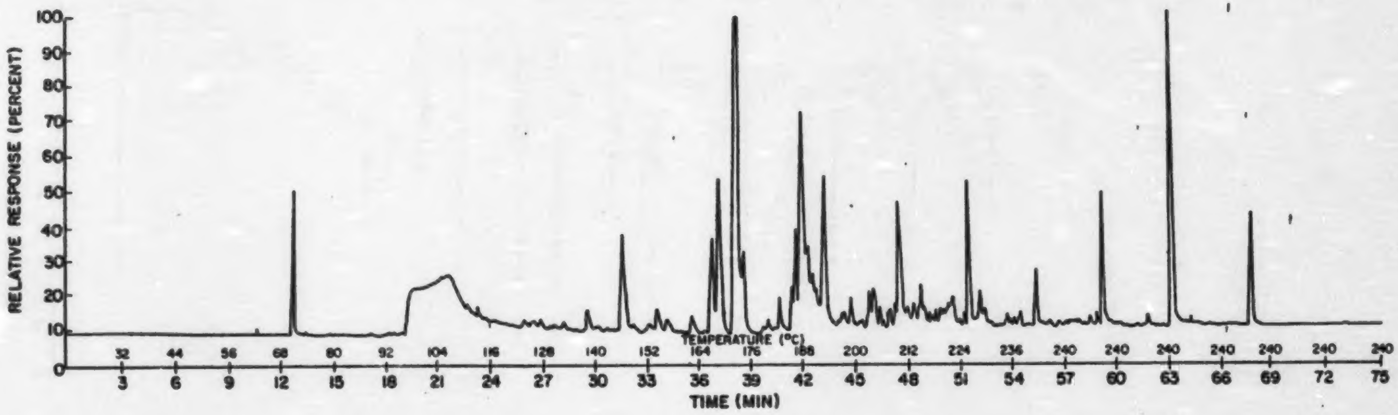


Figure 9. Profile of ambient air pollutants obtained for C. H. Milby Park, Pasadena, TX using capillary gas chromatography/mass spectrometry/computer. A 400 ft S. S. SCOT coated with OV-101 stationary phase was used; temperature programmed from 20-240°C @ 4°C/min.

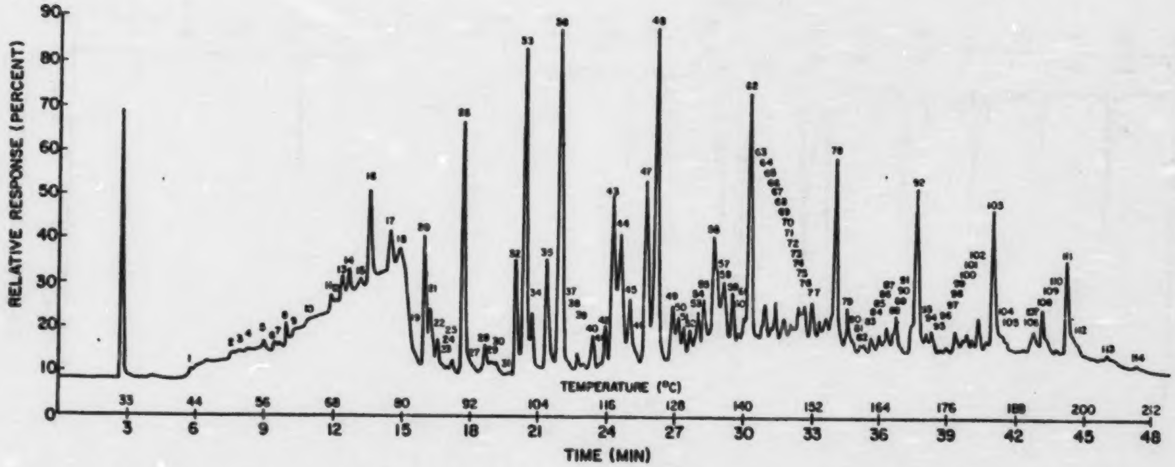


Figure 10. Profile of ambient air pollutants for Wood River, IL, using glass capillary gas chromatography/mass spectrometry/computer. A 42 m glass SCOT coated with OV-101 stationary phase was used; temperature programmed from 20-220°C @ 4°C/min.

SECTION 8

CHARACTERIZATION OF ORGANIC VAPOR EMISSIONS FROM CONTROLLED PRE-SET FIRES

The objective of this study was to apply a new technique which had been developed for ambient air analysis to the identification of any hazardous organic vapors which might be emitted from controlled deliberately set fires of lobbly pine needles. In addition to the identification of organic compounds in emitted vapors, an estimation of the quantities of each of the constituents was made.

EXPERIMENTAL

Sampling Procedure

The sampling procedure employed consisted of concentrating organic vapors on a 1.5 x 10.0 cm glass sampling cartridge containing the sorbent Tenax GC® (35/60 mesh). All sampling cartridges were preconditioned by heating to 275°C for a period of 20 min under a helium purge of 20-30 ml/min. The sorbent used in the sampling cartridges was previously extracted with acetone for a period of 18 hr in a Soxhlet apparatus. The preconditioned sampling cartridges were then cooled in a Teflon®-lined capped Corex® centrifuge tubes to prevent contamination of the cartridge. Sampling cartridges prepared in this manner were carried by automobile to the Southeastern Forest Exprimental Station in Macon, GA for sampling of vapors from fires. Of this group of sampling cartridges, 2-3 cartridges were designated as controls to establish whether contamination occurred by the packing and transportation procedure.

Two portable field samplers (Model 221-A, Nutech Corp., Durham, NC) were used. The portable field samplers were fabricated according to the design criteria as outlined in previous reports which allowed sampling to be conducted in either AC or DC mode.(1) A glass fiber filter (Gelman type A/E) was used to remove particulate material. Organic vapors which passed through the glass fiber filter were collected on the Tenax GC® sampling cartridge.

The experimental protocol for sampling organic vapors emitted from fires is given in Table 5. Two types of fires were set. One was a front fire, the second a back fire. Organic vapors were collected on Tenax GC® cartridges during the flame period and during the smouldering period from each of these fires. The intention was to sample at a point above the flame (n/m) as well as at the roof-top (~3-4 m). Since it began to rain during the first experiment, a sample from the roof-top during the smouldering period was not taken, nor during any of the subsequent experiments. Thus vapors were collected only indoors. In the third experiment the quantity of lobbly pine needles was increased to 6 lbs (head fire).

Characterization of Organics Emitted from Fires

The instrumental system (glc/ms/comp) used for the qualitative analyses of organic vapors and the inlet-manifold used for recovering vapors trapped on Tenax GC® sampling cartridges has been previously described.(1-4)

The operating parameters for the glc/ms/comp system for analysis of samples are shown in Table 6. Samples were analyzed on a 100 m glass SCOT capillary coated with OV-101 stationary phase. The desorption of vapors from the sampling cartridges was achieved at 265-270°C. A single stage glass jet separator interfaced the SCOT capillary columns to the mass spectrometer and was maintained at 220°C. The capillary column was programmed from 20-240°C @ 4°C/min.

Identification of resolved components was achieved by comparing the mass cracking pattern of the unknown mass spectra to an 8 major peak index of mass spectra(12) and to the Wiley collection.(13) In several cases, the identification was confirmed by comparison with authentic compounds of the mass spectrum and the elution temperature. Particular note was made of the relationship of the boiling point of the identified compound to its elution temperature and to the order of elution of the constituents in a homologous series since the OV-101 SCOT capillary column separates primarily on the basis of boiling point. For estimation of the levels of each of the constituents that were identified, the relative molar response was used in order to calculate an approximate value for the concentration of the constituent. The concentration was expressed in ng/ℓ of air sampled above the fire. The concentration was also based upon the breakthrough volume of the constituent for the Tenax GC sampling cartridge.

Table 5. EXPERIMENTAL PROTOCOL FOR SAMPLING ORGANIC VAPORS EMITTED FROM FIRES

Experiment No.	Burn Type/Period	Sampling Point	Sampling Time (min)	Sampling Rate (ℓ/min)	Total Volume/Cartridge (ℓ)
1A	Head fire/flame	above flame	7.5	6.7	50.2
1B	Head fire/smouldering	above flame	12.0	6.2	74.4
1C	Head fire/flame	at roof-top	7.0	4.6	32.2
2A	Back fire/flame	above flame	7.0	5.8	45.2
2B	Back fire/smouldering	above flame	8.0	7.4	59.2
3A	Head fire/flame	above flame	7.0	6.2	43.4
3B	Head fire/smouldering	above flame	20	5.8	116.0

Table 6. OPERATING PARAMETERS FOR GLC-MS-COMP SYSTEM

Parameter	Setting
Inlet-manifold	
desorption chamber	265°-270°
valve	175°
capillary trap - minimum	-195°C
maximum	+175°C
thermal desorption time	~4 min
GLC	
OV-101 glass SCOT (100 m)	20-240°C
carrier (He)	1.5 ml/min
MS	
single stage glass jet separator	200°C
ion source vacuum	~2×10^{-6} torr
filament current	300 μA
multiplier	5.5
scan rate, automatic-cyclic	1 sec/decade
scan range	*m/e* 20 → 300

RESULTS AND DISCUSSION

The results of the experiment No. 1A (Fig. 11) are shown in Table 7. This experiment consisted of a front burn and the sampling was done during the flame period. The total volume collected on the Tenax GC sampling cartridge was 50.2 ℓ. Based upon the absolute quantity on the sampling cartridge as determined by gc/ms/comp analysis and the breakthrough volume for each of the constituents, an estimation was made of the concentration of that vapor per liter of gas sampled. The major constituents emitted from the fire were benzene (320 ng/ℓ), toluene (891 ng/ℓ), furfural (627 ng/ℓ), p-xylene (529 ng/ℓ), and limonene (622 ng/ℓ). As can be seen in Table 7 there were many alkanes, alkenes and in particular oxygenated compounds which were analogs of furan. Also indicated are those compounds which can be regarded as background vapors in the ambient air. Several background peaks which constitute "bleed" from the chromatographic column are also labelled. In many cases where there were peaks which were not homogeneous, the identity of the constituents were designated by an alpha-numeric system. For example, peak No. 3 contained n-butane, isobutane and 2-methylpropene and the latter two were designated 3A and 3B. Also, it is important to note that the numbering sequence is not in all cases complete. Where the chromatographic peak number has been omitted, the identity of the constituent could not be established.

The results of experiment 1B are shown in Table 8. Sampling was performed during the smouldering period, in contrast to the previous case which was during the flame period. This sample contained acetamide and 4 phenols (o-methoxyphenol, o-methallyphenol, phenol and o-cresol).

In experiment 1C (Fig. 12 and Table 9) vapors were collected at the roof-top during the flame period. This sample in contrast to the one presented in Table 8 exhibited a larger number of carbonyl compounds. Also, phenols were not detected during the flame period.

Experiment 2A and 2B represented a repeat of the experiment 1 except a backfire was set. In this case sampling at the roof-top was complicated by rain. When this sample was examined, there was an appreciable amount of water which interferred with the gc/ms/comp analysis. Thus, the identification was possible of only those constituents present in the smouldering sample taken indoors above the fire.

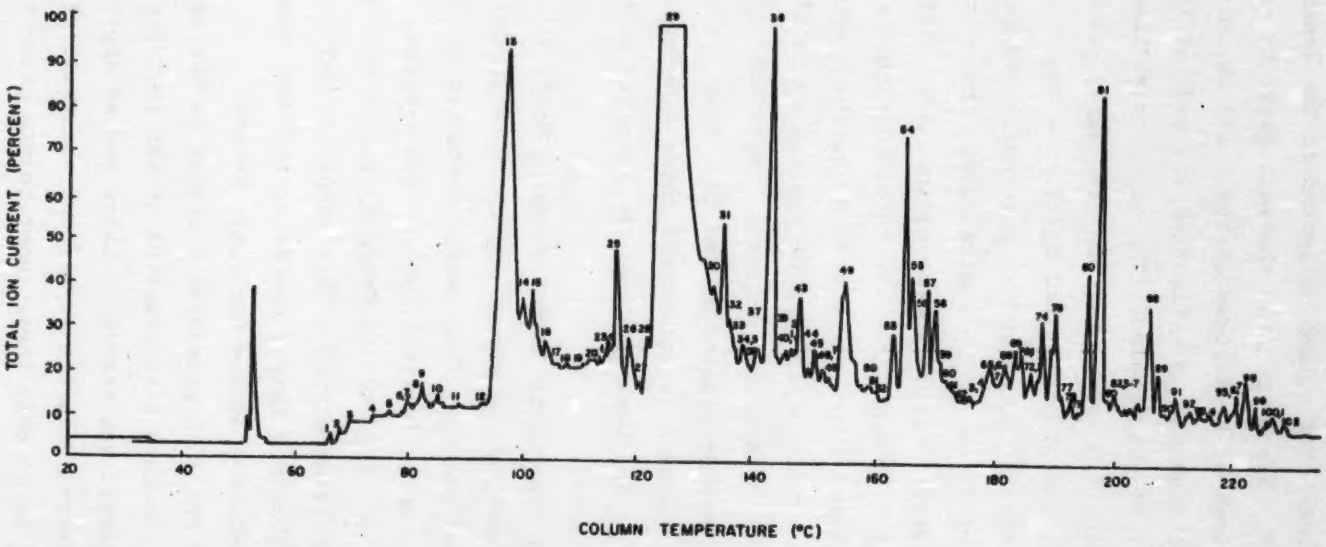


Figure 11. Organic vapor profile for experiment 1A.

Table 7. ORGANIC VAPORS EMITTED FROM HEAD FIRE DURING FLAME PERIOD[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
1	54	unknown	-
2	62	[b]chloromethane	5
3	62	n-butane	2
3A	63	isobutane	1
3B	64	2-methylpropene	-
4	74	1-pentene	-
5	77	isopentane	2
6	79	C_5H_{10} isomer	1
7	80	furan	8
7A	80	C_5H_{10} isomer	1
8	81	n-pentane	2
9	82	acetone	15
9A	82	isoprene	1
10	85	2-methyl-2-butene	6
11	89	cyclopentadiene	2
11A	91	methyl ally ether	-
11B	91	cyclopentane	-
12	92	glycerol	3
13A	94	methoxymethylsilane (BKG)	-
13	94-102	trimethylsilanol (BKG)	-
14	97	diacetyl	17
14A	99	1-hexene	-
15	100	2-pentanone	38
15A	101	2-methylfuran	-
20	102	n-hexane	-
21	109	C_6H_{10} isomer	2
21A	111	C_6H_8 isomer	-

(continued)

Table 7 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
21B	111	[b]1,1,1-trichloroethane	-
23	112	C_6H_{10} isomer	-
24	114	2,4-hexadiene	3
25	116	benzene	320
26	118	2-methyl-4,5-dihydrofuran + C_7H_{16} isomer	(83 + 64)
27	119	2,5-dimethyltetrahydrofuran	5
28	120.5	*n*-heptane	4
29	120-135	BKG peak	-
31	113	C_7H_{14} isomer	-
34	137	3-methylhexane	17
36	139	C_8H_{16} isomer	22
38	141	toluene	891
43	146	1-octene + $C_7H_{10}O$ isomer	129
45	149	*n*-octane	26
46	150	furan-3-aldehyde	5
47	151	2,3,5-trimethylfuran	-
48	152	hexamethyltrisiloxane (BKG)	-
49	153	furfural	627
51	159	C_9H_{16} isomer	-
53	163	ethylbenzene	144
54	165	*p*-xylene	529
55	166-167	BKG peak	-
56	168	1-nonene	219
57	169	styrene	192
58	170	*o*-xylene	144
59	171	*n*-nonane	-
60	171.5	2-isopropylfuran	-

(continued)

Table 7 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
61	172.5	anisole	-
63	175.5	o-methylanisole	-
63A	176	isopropylbenzene	-
66	180	2-methylstyrene	32
68	182	benzaldehyde	18
69	182	5-methyl-2-furaldehyde + p-tolualdehyde	-
70	183	1,3,5-trimethylbenzene	6
71	185	$C_{10}H_{16}$ isomer	9
72	186	α-methylstyrene	19
73	187	$C_{10}H_{18}$ isomer	-
74	189	1-decyne	158
75	189.5	m-methylstyrene	-
76	190.5	m-ethyltoluene	161
77	191	benzofuran	2
77A	192	myrcene	-
78	193.5	dichlorobenzene	16
79	194	2-methyl-5-isopropyl-furan	2
79A	195	o-cymene	-
80	196	1,2,3-trimethylbenzene	232
80A	197	2-n-butyrylfuran	-
81	198.5	limonene	622
82	200	trimethylphenoxysilane (BKG)	-
83	200.5	C_4-alkyl benzene	2
84	201	indene	1
84A	201.5	m-diethylbenzene	-
85	202	n-butylbenzene	-
85A	202.5	1,1,2-trichloropropane (tent.)	-
87	205	1-undecene	3

(continued)

Table 7 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
88	207	unknown	163
89	208.5	*n*-undecane	27
90	209	cyclododecene + *o*-methoxybenzaldehyde	3
91	210	C_5-alkyl benzene	24
91A	211	7-methylbenzofuran	-
91B	212	*o*-methyoxyphenol	-
92	213	*o*-methylacetophenone	6
93	215.5	C_5-alkyl benzene	-
96	220.5	3-methylindene	-
99	225	[b]1,2,4-trichlorobenzene	9
99A	226	*n*-dodecane	-
100	227	naphthalene	4
101	228	dimethyldihydroindene	5
102	230	1-methyl-3-t-butyl-benzene	6
105	236	trimethyldihydroindene	-
108	240.5	1-tridecene	38
109	242	*n*-tridecane	36

[a] See Tables 5 and 6 for sampling and instrumental conditions, expt. 1A.

[b] Vapors often present in ambient air sampled.

Table 8. ORGANIC VAPORS EMITTED FROM HEAD FIRE DURING SMOULDERING PERIOD[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
2	68	1-pentene	3
2A	72	C_5H_{12} isomer	-
3	75	isopentane	1
3A	76	C_5H_{10} isomer	-
3B	77	furan	-
3C	77	2-pentene	-
4	78	n-pentane	2
5	79	isoprene	2
5A	80	diethyl ether	-
5B	81	acetone	-
6	82	2-methyl-2-butene	2
6A	86	dimethoxymethane	-
6B	87	unknown	-
6C	90	cyclopentene	-
6D	91	ethyl vinyl ether	-
7	92	column background	-
8	93	column background	-
8A	94	diacetyl	-
8B	95	C_6H_{14} isomer	-
9	96	1-hexene	2
10	98	2-methylfuran	12
11	99	n-hexane	3
12	100	[b]chloroform	4
13	103	3-methyl-2-pentene	-
14	104	3-methylpentane	-
15	105	methylcyclopentane	-
15A	106	C_6H_{10} isomer	-
15B	107	1,3,5-hexatriene	-
15C	108	C_6H_{12} isomer	-

(continued)

Table 8 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
16	108	[b]1,1,1-trichloroethane	1
16A	109	$C_5H_{10}O$ isomer	-
16B	110	2,4-hexadiene	-
17	111	2-pentanone	-
18	112	benzene	77
18A	113	[b]carbon tetrachloride	-
19	114	C_7H_{16} isomer	27
20	115	2,4-dimethylpentane	21
20A	115	3-methyl-hexane	-
21	116	C_7H_{14} isomer	18
22	117	cycloheptane	-
22	116-129	hexamethyldisiloxane (BKG)	-
24	120	2,5-dimethylfuran	8
25	121	n-heptane	29
26	122	2-vinylfuran	-
27	125	cyclohexylamine (tent.)	-
28	127	dimethylpentene isomer	6
29	129	2-hexenal	92
30	132	2-ethyl-1-hexene	11
31	134	1,trans-2,cis-3-trimethylcyclopentane	9
32	137	toluene	97
33	139	1-octene	6
35	142	trans-4-octene	7
35A	143	C_8H_{14} isomer	-
35B	144	2-octene	-
36	145	n-octane	9
37	146	2,3,5-trimethylfuran + furan-3-aldehyde	(2 + 1)
38	148	hexamethylcyclotrisiloxane (BKG)	-

(continued)

Table 8 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
39	149	2-methyl-5-vinylfuran	2
40	152	furfural	31
40A	153	2,5-diethylfuran	-
41	159	ethylbenzene	8
42	161	*p*-xylene	101
42A	161	C_9H_{18} isomer	-
43	162	octamethyltrisiloxane (BKG)	-
44	165	1-nonene	7
44A	165	styrene	-
45	166	*o*-xylene	22
46	167	*n*-nonane	3
46A	168	C_9H_{18} isomer	-
47	169	furyl methyl ketone	-
48	172	isopropylbenzene	-
50	178	$C_{10}H_{16}$ isomer	-
50A	178.5	*m*-ethyltoluene	-
51	179	5-methyl-2-furaldehyde + benzaldehyde	-
52	181	*p*-ethyltoluene	111
53	180-4	acetamide	123
54	183	*o*-ethyltoluene	96
56	185	α-methylstyrene + 1-decene	-
57	187	1,3,5-trimethylbenzene + $C_{10}H_{18}$ isomer	9
57A	188	*n*-decane	-
61	193	*o*-cymene	31
61A	193	1,2,3-trimethylbenzene	33
62	194	$C_{10}H_{18}$ isomer	75
62A	195	limonene	-
63	196	*p*-propyltoluene	-

(continued)

Table 8 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
64	198	indene	-
65	199	1,2-diethylbenzene	2
66	201	acetophenone	4
68	204	1-undecene	12
68A	205	unknown	-
69	206	*n*-undecane	11
70	207	2-methylbenzofuran	-
71	210	dimethylethylbenzene (isomer ?)	4
72	212	C_4-alkyl benzene	15
72A	213	*o*-methoxyphenol	14
72B	214	*o*-methallylphenol	-
75	220	cyclododecane	2
76	221	unknown	-
77	223	*n*-dodecane	7
77A	224	trimethylphenoxysilane (BKG)	-
78	225	phenol	49
78A	226	naphthalene	-
79	227	*o*-cresol	11
82	237	$C_{13}H_{26}$ isomer	-
83	239	$C_{13}H_{26}$ isomer	2
84	241	*n*-tridecane	4

[a] See Tables 5 and 6 for sampling and instrumental conditions, expt. 1B

[b] Vapors often observed in ambient air.

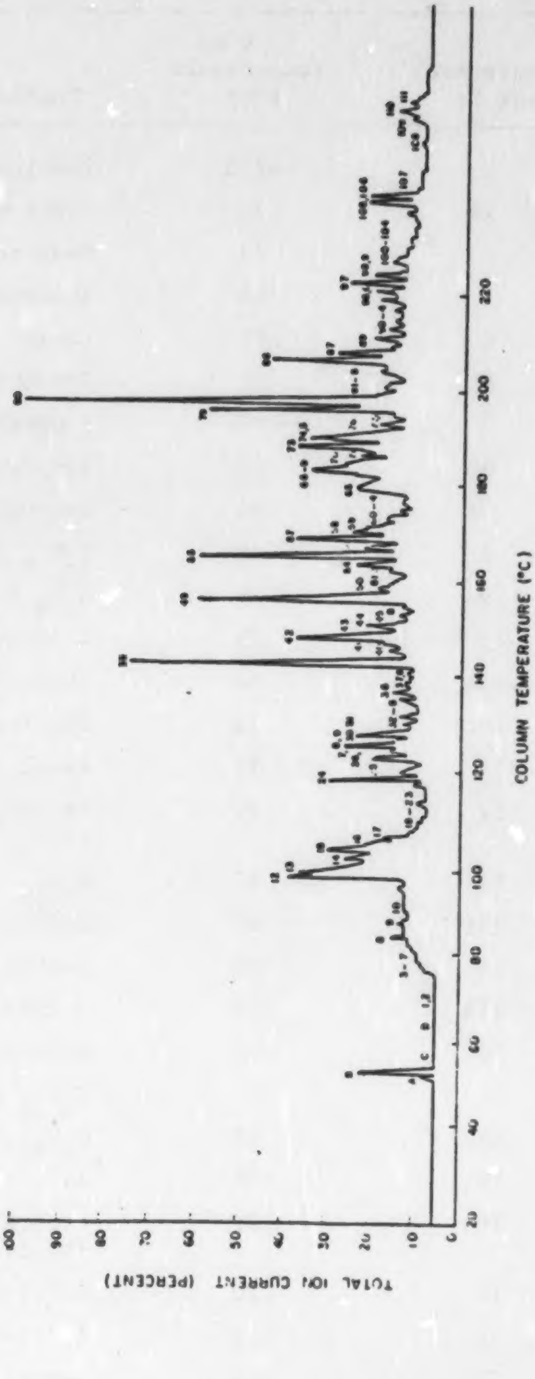


Figure 12. Organic vapor profile for experiment 1C.

Table 9. ORGANIC VAPORS EMITTED FROM HEAD FIRE DURING FLAME PERIOD[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
2	67.5	2-chloropropane	-
2A	72	1-butene	-
4	78	isopentane	-
5	80	1-pentene	-
6	81	furan	2
6A	81	2-methyl-2-butene	-
7	82	*n*-pentane	3
8	83	isoprene	21
8A	84	acetone	-
9	86	C_5H_{10} isomer	15
9A	88	C_5H_8 isomer	-
10	89	1,3-pentadiene	7
10A	90	cyclopentadiene	-
10B	91	SO_2 (tent.)	-
11	93	vinyl ethyl ether	8
12	96	isopropanol + trimethyl silanol (BKG)	15 (alcohol)
13	97	C_6H_{14} isomer	23
13A	98	methyl vinyl ketone	-
14	101	methyl cyclopentane	45
14A	101	methyl ethyl ketone	-
15	102	2-methyl furan	97
17	104	C_6H_{12} isomer	7
18A	107	C_6H_{10} isomer	-
18	108	[b]1,1,1-trichloroethane	3
18B	109	methyl propionate (tent.)	-
19	110	2,4-hexadiene	10
20	112	1,3,5-hexatriene	15
21	114	3-methylbutanal (tent.)	9
22	115	C_6H_{10} isomer	8

(continued)

Table 9 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
23	116	methyl isopropyl ketone	33
24	117	benzene	330
24A	118	C_6H_{12} isomer	-
25	118-120	methyl isopropenyl ketone	50
26	121	2-methyl-3-pentanone	54
27	122	2,4-dimethylpentane	12
28	124	unknown	-
29	125	1-trans-2-dimethylcyclopentane	240
30	125	2-methyl-2,4-hexadiene (tent.) or C_7H_{12} isomer	-
30A	126	2,5-dimethylfuran	-
31	127	n-heptane	280
32	128	trans-2-heptene	-
33	129	2,4-dimethylfuran	3
34	130	2-vinylfuran	21
34A	131	C_7H_{12} isomer	-
35	134	methylcyclohexane	24
35A	134.5	2-methyl-4,5-dihydrofuran	-
36	135	dihydropyran (tent.)	23
36A	136	furan-3-aldehyde	-
37	137	C_7H_{12} isomer	4
38	140	3-ethyl-2-pentene	8
39	142	toluene	704
40	144	C_7H_{12} isomer	22
41	146	1-methylcyclohexadiene	15
42	147	1-octene	321
44	150	n-octane	25
45	151	2,3,5-trimethylfuran	7

(continued)

Table 9 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
47	152	hexamethylcyclotrisiloxane (BKG)	-
49	155-157	furfural	2096
54	163	ethylbenzene	301
55	165	p-xylene	659
56	166	1-nonene	32
57	169	styrene	348
58	170	o-xylene	25
59	171	n-nonane	13
60	172	2-isopropylfuran (tent.)	-
61	173	anisole	27
62	174	furyl methyl ketone (tent.)	5
63	176	2-isobutenylfuran or o-methylanisole	-
64	177	isopropylbenzene	4
66	180	n-propylbenzene	-
67	182	5-methyl-2-furfural + benzaldehyde	-
68	183	C_9H_{12}	-
69	184	1,3,5-trimethylbenzene	21
70	185	$C_{10}H_{16}$ isomer	-
71	186	$C_{10}H_{18}$ isomer	26
73	188	$C_{10}H_{20}$ isomer	342
74	190	α-methylstyrene	-
75	191	C_3-alkyl benzene	419
76	192	benzofuran	-
77	193	$C_8H_{10}O$ + $C_{10}H_{16}$ isomers	89
78	195	1-decene	-
79	196	o-cymene	-
79A	196	1,2,3-trimethylbenzene	-

(continued)

Table 9 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
79B	197	2-n-butyrylfuran	-
80	198	$C_{10}H_{16}$ isomer	-
80A	199	limonene	-
81	199.5	unknown	-
82	201	indene	17
83	202	diethylbenzene	14
84	204	C_4-alkyl benzene	11
85	205	1-undecene	12
86	206-7	unknown	-
87	208	n-undecane	115
87A	208	1-methyl-4-isopropenylbenzene	-
88	209	C_5-alkyl benzene	12
95	220	methyl indene	47
97	223	cyclododecane	132
98	225	n-dodecane	96
100	228	naphthalene	76
101	230	4,7-dimethylbenzofuran	6
104	238	$C_{13}H_{24}$ isomer	-
105	240	1-tridecene	107
106	242	n-tridecane	109
107	245	biphenyl	-
110	261	1-tetradecene	145
111	263	n-tetradecane	86

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[a] See Tables 5 and 6 for sampling and analysis conditions, expt. 1C.

[b] Vapors often observed in ambient air.

Table 10 lists the organic vapors identified for Experiment 2A. Again the major constituents were benzene, toluene, and xylene. In this sample a trace of acetaldehyde was detected. This experiment produced a fewer number of oxygenated compounds during the flame period as compared to experiment 1A. The majority of vapors emitted during the smouldering period (Expt. 2B, Table 11) were alkanes and alkenes (straight and branched).

Tables 12 and 13 list the compounds identified from the flame and smouldering period, respectively, of a head fire for a 6 lb. load of pine needles. This experiment was not as successful since there had been larger accumulation of fine carbon-like particles which passed through the glass fiber filter and settled in the Tenax GC sorbent bed. The presence of carbon apparently complicated the desorption of organic vapors from the cartridge. The overall quantity of each organic compound was considerable less than expected for the increased pine needle load (compared to Expt. 1A and 1B).

Future studies of this nature which utilized a Tenax GC sampling cartridge can be improved by:

(1) employing a glass fiber filter (or equivalent) which will retain fine carbon particles generated during burning,

(2) reducing the total volume of air sampled in order to avoid overloading the glass capillary column used for resolving the mixture of components,

and (3) sampling at ambient temperature of 50-70°C instead of cooling the cartridge with ice in order to minimize accumulation of water.

Table 10. ORGANIC VAPORS IDENTIFIED IN EMISSIONS FROM BACKFIRE DURING FLAME PERIOD[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
1	68	acetaldehyde	–
1A	72	isopentane	–
1B	73	[b]trifluoromethane	–
1C	74	1-pentene	–
2	77	furan	4
2A	76	1,3-pentadiene	3
3	81	acetone	3
3A	82	divinyl ether	–
3B	82	[b]methylene chloride	–
3C	84	methylal (tent.)	–
3D	86	cyclopentadiene (tent.)	–
3E	88	carbon disulfide	–
4	92	dihydrofuran + C_6H_{12} isomer	3
4A	92	2-methylprop-2-en-1-al	–
4B	93	trimethyl silanol (BKG)	–
4C	94	diacetyl	–
4D	96	C_6H_{12} isomer	–
5	96	methylcyclopentane	4
6	97	2-methylfuran + methyl vinyl ketone	4
6A	98	2-methylpentane	–
6B	98	methyl ethyl ketone	–
7	100	[b]chloroform	7
7A	102	3-methyl-2-pentene	–
10	108	[b]1,1,1-trichloroethane	3
11	112	benzene	252
11A	113	[b]carbon tetrachloride	–
13	115	4-methyl pentane	8

(continued)

Table 10 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
14	116	1-cis-3-dimethylcyclopentane	16
14A	117	3-ethylpentane	3
14B	118	3,4-dimethyl-1-pentene	-
16	120	2,3-dihydrofuran	4
17	122	1-trans-2-dimethylcyclopentane	13
17A	122	2,5-dimethylfuran	-
17B	123	n-heptane	-
17C	124	2,4-dimethylfuran	-
18	126	2-vinylfuran	2
19	127	2,2,4-trimethylpentane	9
20	129	methyl cyclohexane	200
21	130	2,4-dimethylhexane	-
22	131	2,2,3-trimethylpentane	-
23	132	C_7H_{16} isomer	10
23A	133	1-cis-2,cis-3-trimethyl cyclopentane	-
24	134	methyl propenyl ketone	6
24A	135	1-trans-2,cis-3-trimethyl cyclopentane	-
24B	135	C_7H_{14} isomer	-
25	136	toluene	1021
26	137	C_8H_{18} isomer	8
27	142	C_8H_{16} isomer	19
28	144	n-octane	4
30	147	hexamethylcyclotrisiloxane (BKG)	-
31	148	furfural	87
32	150	3-furaldehyde	3
34	157	ethylbenzene	79
35	158-9	p-xylene	338

(continued)

Table 10 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
37	163	styrene	99
38	164	*o*-xylene	92
39	166	*n*-nonane	-
39A	167	2-iso-propylfuran (tent.)	-
39B	168	anisole	-
40	170	isopropylbenzene	2
42	174	5-methyl-2-furaldehyde	2
43	175	unknown	-
44	177	*o*-ethyltoluene	7
46	178	phenylisocyanid or 2-ethenyl-pyridine (tent.)	-
47	179	α-methyl styrene	-
48	180	C_4-alkyl benzene	-
50	182	1-decene	18
51	183	*m*-methylstyrene	4
52	184	1,3,5-trimethylbenzene	57
53	185	benzofuran	-
53A	186	$C_{10}H_{16}$ isomer	-
54	187	[b]*m*-dichlorobenzene	3
55	189	*o*-cymene	80
55A	189	1,2,3-trimethylbenzene	-
55B	190	2-decyne	-
56	191	limonene	92
57	193	2,3-dihydroindene (tent.) + C_9H_{10} isomer	-
58	194	indene	5
59	200	unknown	-
60	202	unknown	-
61	203	unknown	-
62	203	$C_{10}H_{12}$ isomer	8

(continued)

Table 10 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
62A	204	*n*-undecane	-
64	205	2-methylbenzofuran	-

[a] See Table 5 and 6, expt. 2A.

[b] Probably background in ambient air.

Table 11. ORGANIC VAPORS EMITTED FROM BACK FIRE DURING FLAME PERIOD[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
5	98	2-methylpentane	-
6	101	trimethylsilanol (BKG)	-
7	102	1-hexene	1
8	104	2-methylfuran	1
9	105	C_6H_{14} isomer	2
10	106	[b]chloroform	5
11	110	n-hexane	2
11A	111	2,2,3-trimethylbutane	-
12	112	2-methyl-1-pentene	2
13	114.5	3-methylpentane	3
13A	115	[b]1,1,1-trichloroethane	-
13B	115	unknown	-
13C	116.5	2,4-hexadiene	-
13D	117	3-methylcyclopentane	-
14	117.5	benzene	25
15	119.5	carbon tetrachloride	-
15A	119.5	2,4-dimethyl-1-pentene	-
16	120.5	cyclohexane	20
17	122	3-ethylpentane	13
18	122.5	3,4-dimethyl-1-pentene	20
19	126	[b]trichloroethylene	18
20	127	1-trans-2-dimethyl-cyclopentane	19
21	127.5	n-pentane	23
21A	131.5	2-vinylfuran	-
23A	134.5	1,3-dimethylcyclopentane	-
23	135.5	2,3-dimethyl-2-pentene	82
24	136	C_9H_{20} isomer	-
25	137	4,4-dimethyl-1-pentane	-

(continued)

Table 11 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
26	138	C_7H_{16} isomer	19
26A	139	1-cis-2,cis-3-trimethylcyclopentane	-
27	140	1-trans-2,cis-3-trimethylcyclopentane	5
28	142-144	toluene	240
29	144-145	3,4-dimethylhexane	6
30	148	1-trans-2-dimethylcyclohexane	7
31	149.5	1,1-dimethylcyclohexane	4
31A	149.5	*n*-octane	-
32	152	hexamethylcyclotrisiloxane (BKG)	-
33	162-163	ethylbenzene	20
34	164-166	*p*-xylene	76
35	168	styrene	6
36	170	*o*-xylene	40
37	180-181	terpene	1
38	182	n-propylbenzene	1
38A	182	benzaldehyde	-
39	183	*p*-ethyltoluene	-
40	184	$C_{10}H_{22}$	-
41	185-186	phenyl isocyanid or 3-ethyl-pyridine	-
42	187	1,3,5-trimethylbenzene	-
43	188.5	4-methylstyrene	-
44	190	2,3-benzofuran	7
44A	193	[b]*m*-dichlorobenzene	-
45	195	*o*-cymene	6
45A	195	1,2,3-trimethylbenzene	5
46	197.5	limonene	4
46A	198.5	α-methylstyrene	-

(continued)

Table 11 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound	ng/ℓ
46B	200	indene	-
46C	200	_p_-diethylbenzene	-
50	207-208	_n_-undecane	3
54	222	1-dodecene	1
56	224	_n_-dodecane	1
58	225-227	naphthalene	3
61	260	4-methylazobenzene	2

[a] See Tables 5 and 6, expt. 2B.

[b] Probably background vapors in ambient air.

Table 12. ORGANIC VAPORS IDENTIFIED IN EMISSIONS FROM BACKFIRE DURING FIRE PERIOD

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1-4	-	unknowns
5	98	2-methylpentane
6	101	trimethylsilanol (BKG)
7	102	1-hexene
8	104	2-methylfuran
9	105	C_6H_{14} isomer
10	106-7	[b]chloroform
11	110-111	_n_-hexane
11A	111	2,2,3-trimethylbutane
12	112	2-methyl-1-pentene (tent.)
13	114.5	3-methylpentane
13A	115	[b]1,1,1-trichloroethane
13B	115	C_7H_8 (?)
13C	116.5	2,4-hexadiene
13D	117	3-methylcyclopentane
14	117.5-119	benzene
15	119.5	[b]carbon tetrachloride
15A	119.5	2,4-dimethyl-1-pentene
16	120.5	cyclohexane
17	122	3-ethylpentane
18	122.5	3,4-dimethyl-1-pentene
19	126	[b]trichloroethylene
20	127	1-trans-2-dimethylcyclopentane
21	127.5	_n_-heptane
21A	131.5	2-vinylfuran
23A	134.5	1,3-dimethylcyclopentane
23	135.5	2,3-dimethyl-2-pentene
24	136	C_9H_{20} isomer
25	137	4,4-dimethyl-1-pentene
26	138	C_7H_{16} isomer

(continued)

Table 12 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
26A	139	1-cis-2,cis-3-trimethylcyclopentane
27	140	1-trans-2,cis-3-trimethylcyclopentane
28	142-144	toluene
29	144-145	3,4-dimethylhexane
30	148	1-trans-2-dimethylcyclohexane
31	149.5	1,1-dimethylcyclohexane
31A	149.5	n-octane
32	152	hexamethylcyclotrisiloxane (BKG)
33	162-3	ethylbenzene
34	164-6	p-xylene
35	168	styrene
36	170	o-xylene
37	180-1	terpene
38	182	n-propylbenzene
38A	182	benzaldehyde
39	183	p-ethyltoluene
40	184	$C_{10}H_{22}$ isomer
41	185-6	phenylisocyanid or 3-ethenylpyridine (tent.)
42	187	1,3,5-trimethylbenzene
43	188.5	4-methyl-styrene
44	190	2,3-benzofuran
44A	193	m-dichlorobenzene
45	195	o-cymene
46	197.5	limonene
46A	198.5	α-methylstyrene
46B	200	indene

(continued)

Table 12 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
46C	200	_p_-diethylbenzene
50	207-8	_n_-undecane
54	222	1-dodecene
56	224	_n_-dodecane
58	225-7	naphthalene
61	260	4-methylazoebenzene (tent.)

[a] See Tables 5 and 6, expt. 3A.

[b] Probably background vapors from ambient air.

Table 13. ORGANIC VAPORS EMITTED FROM PINE NEEDLES DURING SMOULDERING PERIOD[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	65	C_4H_8
2	74	isopentane
2A	75	[b]trichlorofluoromethane
2B	77	1-pentene
2C	78	furan
2D	78	C_5H_{10}
3	79	*n*-pentane
3A	79	isoprene
3B	81	acetone
4	83	C_5H_{10} isomer + [b]methylene chloride
4A	84	isopropanol
4B	85	cyclopentadiene
4C	86	[b]carbon disulfide (tent.)
5	89	C_6H_{12} isomer
6	92-3	3-methyl-2-pentene + 2-methylpentane
6A	94	[c]trimethylsilanol (BKG)
7	94	diacetyl
7A	97	C_6H_{12} isomer
8	97	1-hexene
8A	98	methyl vinyl ketone
9	99	2-methylfuran
10	99	*n*-hexane
10A	101	trans-methyl propenyl ketone (tent.)
11	102	chloroform
12	104	pent-2-en-4-one
13	105	1-methylcyclohexane
13A	106	2,2,3-trimethylbutane
14	107	2,2-dimethylpentane
15	105	2,4-hexadiene

(continued)

Table 13 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
16	110	1,3,5-hexatriene
16A	111	1,1,1-trichloroethane
17	112	3-methylbutanal
19	114	C_6H_{14} isomer
20	115	benzene
20A	116	[b]carbon tetrachloride
21	117	cyclohexane
21A	117	2-methylpent-1-en-3-one (tent.) + C_7H_{16} isomer
22	118	4-methylpentene
23	119	2,4-dimethylpentane
24	122	1-trans-2-dimethylcyclopentane
24A	123	sorbaldehyde (tent.)
25	124	[b]trichloroethylene
26	125	2,5-dimethylfuran
26A	125	n-heptane
27	126	cis-2-heptane
28	127	2,4-dimethylfuran
29	129	2-vinylfuran
30	131	C_8H_{14} isomer
30A	131	2-ethylfuran (tent.)
31	133	2,3-dimethyl-2-pentane
32	134	2,4-dimethylhexane
32A	134	methyl cyclopropyl/ketone (tent.)
33	136	1-methyl-1,3-cyclohexadiene (tent.)
34	137	C_8H_{16} isomer
35	139	C_7H_{12} isomer
36	141	toluene
37	143	C_8H_{18} isomer
38	144	C_7H_{12} isomer

(continued)

Table 13 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
39	145	1-octene
40	147	2,3-dimethylhexa-1,4-diene
41	148	n-octane
42	150	2,3,5-trimethylfuran
43	152	ᶜhexamethylcyclotrisiloxane (BKG)
44	153	furfural
45	156	C_8H_{14} isomer
46	158	2,5-diethylfuran (tent.) + C_9H_{16} isomer
47	161	C_9H_{18} isomer
48	162	isobutyl acetate (tent.)
49	162	ethyl benzene
50	165	p-xylene
50A	166	2-propionylfuran (tent.)
51	167	C_9H_{18} isomer
52	168	styrene
53	169	o-xylene
54	170	n-nonane + 2-isopropylfuran
55	172	anisole
56	174	2-methyl-5-isopropenylfuran
57	176	cumene
57A	177	$C_8H_{18}O$
58	177	n-decane
59	180	camphene (tent.)
60	182	n-propylbenzene
61	183	m-ethyltoluene
62	183	p-ethyltoluene
63	184	$C_{11}H_{24}$ isomer
64	186	$C_{10}H_{18}$ isomer
65	187	C_3-alkyl benzene

(continued)

Table 13 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
66	188	1-decene
67	191	benzofuran
68	191	$C_{10}H_{22}$ isomer
70	195	_n_-propyltoluene
71	197	_m_-diethylbenzene
72	198	limonene
74	201	_n_-butylbenzene
75	203	_p_-propyltoluene
76	205	dimethyl ethyl benzene (isomer ?)
77	207	_p_-α-dimethylstyrene
78	208	_n_-undecane
87	223	$C_{12}H_{24}$ (cyclododecane ?)
88	225	_n_-dodecane

[a] A 100 m glass SCOT capillary coated with OV-101 stationary phase was used to separate organic vapors. Capillary was temperature programmed from 20-230°C @ 4°/min. Helium flow was 1.7 ml/min.

[b] These vapors have been commonly found in ambient air samples and may be regarded as background in the air itself.

[c] Background from stationary phase "bleed" from glass capillary.

SECTION 9

IDENTIFICATION AND QUANTITATION OF N-NITROSODIMETHYLAMINE IN AMBIENT AIR BY CAPILLARY GAS-LIQUID CHROMATOGRAPHY MASS SPECTROMETRY COMPUTER

In the period from 1950-1969, cancer statistics indicate that the incidence of death from certain types of cancer for Baltimore City and adjacent Anne Arundel County are higher than the comparable rates for either the state of Maryland or the continental United States (see Table 14).[14] Exposure to any known carcinogen usually initiates an induction period for several years before any effect is seen. The higher rates for cancer mortality in areas of the respiratory system for these localities suggest that airborne carcinogens may play an important role, at least in the Baltimore City/Anne Arundel County area. The potency of N-nitrosodimethylamine (DMN) as a carcinogen has been established repeatedly in experimental studies on mice, hamsters, guinea pigs, rats, mink, rabbits and several species of fish.(15) Inhalation of DMN has produced tumors of the nasal area in rats.(15) NIOSH concludes that in view of this broad spectrum of

Table 14. CANCER MORTALITY STATISTICS[a]

	Deaths per 100,000 population			
Type	Baltimore City	Anne Arundel Co.	Maryland	United States
Tongue, mouth	7.3	6.2	5.54	4.21
Esophagus	7.0	5.8	4.94	4.10
Trachea, bronchus, lung	61.1	51.0	48.46	37.98
Nasopharynx	0.9	0.1	0.48	0.38

[a] Statistics for white males.

carcinogenic activity in experimental animals, N-nitrosodimethylamine must be regarded as potentially carcinogenic for man. Notwithstanding the potency of DMN as a carcinogen, it is extremely unlikely that this compound alone could be responsible for a high incidence of cancers since many hazardous agents are introduced to the environment by industrial processes.(16)

Previous analysis of the air in the area of Baltimore City utilized a specific detection method for DMN.(17) Samples were collected cryogenically and analyzed on a thermal energy analyzer (Thermo-Electron, Model 502).(17) Immediate and unequivocal identification of the molecular structure of DMN was not possible by this technique; comparison with a standard was necessary for empirical identification.

Under this research program, the emphasis has been upon obtaining a complete characterization of organic vapors present in the ambient atmosphere to provide a chemical basis for epidemiological studies. This section presents the first report of the unequivocal identification by gc/ms computer of N-nitrosodimethylamine in ambient air in Baltimore, Maryland.

In addition to identifying organic vapors present in the ambient atmosphere,(1,2,18) analysis by the same technqiues developed in this laboratory has provided quantitative information. This section also describes the quantification of N-nitrosodimethylamine in ambient air in Baltimore, MD and the Kanawha Valley, WV using single ion monitoring (m/e 74) in conjunction with glass capillary gas-liquid chromatography/mass spectrometry. Estimation of DMN levels in ambient air was performed in several locations surrounding the FMC site in Baltimore, MD, and Union Carbide and DuPont in the Kanawha Valley.

EXPERIMENTAL

Sampling and Analysis

Organic vapors were concentrated on a 1.5 x 6.0 cm bed of Tenax GC (35/60) in a glass cartridge.(1) All sampling cartridges were preconditioned by heating to 275°C for a period of 20 min under a helium purge of 20-30 ml/min. After cooling in precleaned Kimax® culture tubes, the containers were sealed to prevent contamination of the cartridge. Sampling cartridges prepared in this manner were carried by automobile or air freight to the sampling site; 2-3 cartridges were designated as blanks to determine whether any of the cartridges might have been contaminated by the packing and transportation procedure. Cartridges containing known quantities (100 and 300 ng) of N-nitrosodimethylamine were prepared and carried to and from the field, stored and analyzed to determine recovery of N-nitrosodimethylamine.

In conjunction with Dr. L. Ballard of Nutech Corp. (Durham, NC), portable field samplers were custom-built to operate conveniently and reliably under varying conditions of pressure and gas flow. Precise measurement and regulation were essential.(1) A schematic of the vapor collection and analytical system is depicted in Fig. 13.

Samples taken in replicate, as well as the blanks discussed above, were subjected to analysis by a capillary gas chromatograph/mass spectrometer/computer (Fig. 13). Thermal desorption was used to transfer the entire amount of trapped vapors from the cartridge sampler to the analytical system and required a specially designed manifold.(1-4) In a typical thermal desorption cycle, a sampling cartridge was placed in the preheated (ca. 250°C) desorption chamber, and helium gas was channeled through the cartridge (ca. 20 ml/min) to purge the vapors into the liquid nitrogen cooled nickel capillary trap. After desorption, the six-port valve was rotated and the temperature on the capillary loop was rapidly raised (>10°C/min); the carrier gas introduced the vapors onto the glc column.

A Varian MAT CH-7 glc/ms/comp system was used to perform the analysis (Fig. 13). Mass spectra and retention time data were accumulated on magnetic tape and subsequently processed by a Varian 620/L computer. A reconstructed gas chromatograph provided a correlation between mass spectrum number and retention time. Operating parameters used on the glc/ms/comp system for analysis of samples collected on glass cartridges from the Baltimore, Maryland and Kanawha Valley areas, are shown in Table 15. Ambient air samples were analyzed on 55, 80 or 100 m glass SCOT columns coated with either DEGS, OV-101 or OV-225 stationary phase, respectively. Desorption of ambient air pollutants (including nitrosamines) from the Tenax cartridges was achieved at 265-270°C. A single stage glass jet separator interfaced the SCOT capillary columns to the mass spectrometer and was maintained at 220°C.

Identification of DMN was achieved by comparison of the mass spectrum to an eight peak index of mass spectra(12) and to the Wiley library collection.(13) Identification was confirmed by comparison of mass spectra and

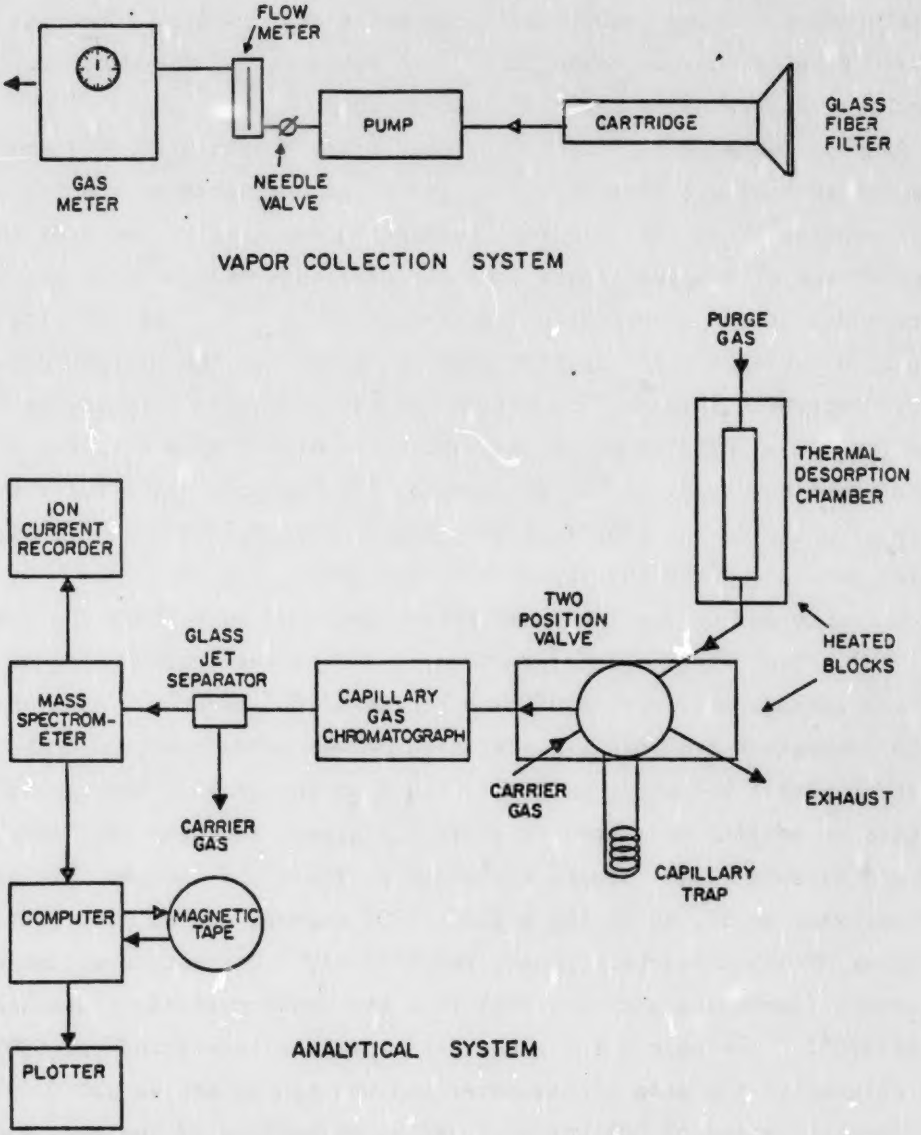

FLOW METER
GAS METER
NEEDLE VALVE
PUMP
CARTRIDGE
GLASS FIBER FILTER
VAPOR COLLECTION SYSTEM
PURGE GAS
THERMAL DESORPTION CHAMBER
HEATED BLOCKS
TWO POSITION VALVE
ION CURRENT RECORDER
GLASS JET SEPARATOR
MASS SPECTROM-ETER
CAPILLARY GAS CHROMATOGRAPH
CARRIER GAS
EXHAUST
CARRIER GAS
CAPILLARY TRAP
COMPUTER
MAGNETIC TAPE
PLOTTER
ANALYTICAL SYSTEM

Figure 13. Vapor collection and analytical systems for analysis of hazardous vapors in ambient air.

Table 15. OPERATING PARAMETERS FOR GLC/MS COMPUTER SYSTEM

Parameter	Setting
Inlet-manifold	
Desorption chamber	265-270°C
Valve	175°C
Capillary trap - minimum	-195°C
maximum	+175°C
Thermal desorption time	~4 min
Gas-liquid Chromatography	
OV-101 glass SCOT (100M)	30-225°C, 4°C/min
OV-225 glass (80M)	80-210°C, 4°C/min
DEGS glass SCOT (55M)	70-205°C, 4°C/min
Carrier (He)	1.5 ml/min
Mass Spectrometry	
Single stage glass jet separator	220°C
Ion source vacuum	~2 x 10^{-6} Torr
Filament current	300 μA
Multiplier	5.5
Scan rate, automatic-cyclic	1 s/decade
Scan range	m/e 20 → 300

elution temperature on two different columns of DMN and an authentic sample (Table 15).

Determination of Breakthrough Volume

Breakthrough volumes for DMN, NO, NO_2, and water were determined as previously described.(19) The vapor was injected onto a gas chromatographic column packed with the sorbent Tenax GC and the elution volume determined at a series of decreasing temperatures. The log of elution volume vs temperature was plotted and the breakthrough volume at ambient temperature (50-90°F) was obtained by extrapolation. The volume of air sampled was less than the breakthrough volume of DMN at the ambient temperature of sampling which allowed quantitative collection.

In Situ Formation of DMN

In order to determine whether DMN may form in an atmospheric chemical reaction it is first necessary to know the extent to which it may be formed at trace levels as an artifact of the sample collection process. Since the Tenax cartridge would concentrate dimethylamine (DMA) if present in ambient air, it was conceivable that, in the presence of NO_x, DMA might be nitrosated to form DMA. Several laboratory and field experiments were conducted to determine whether an in situ reaction could occur on the sampling cartridge. In the first set of experiments, Tenax cartridges were prepared by drawing through them 50 liters of air containing 5 ppm DMA. Then seven liters of a synthetic mixture of NO, water vapor and air (1, 10 or 250 ppb NO, 72% relative humidity) were drawn through the cartridges. The DMA was purified prior to use by low temperature vacuum distillation since it had been found to contain 10 ppm of DMN.

In a second set of experiments, 1, 5, and 10 ppm mixtures of NO in air were introduced into a stream of laboratory air drawn at a rate of 10 liter/min across a permeation tube(6) containing DMA (~9 x 10^{-6} moles/min, 4.5 ppm) and into a Tenax GC cartridge. A third set of experiments consisted of introducing equivalent amounts of NO and NO_2 into an air sampling stream drawn across a DMA permeation tube (4.5 ppm) and into the Tenax cartridge. All the cartridges were analyzed by single ion monitoring (m/e 74) in the capillary glc-ms mode.

Additional experiments were conducted during field sampling at the Baltimore, MD industrial site to determine whether an enhancement in the concentration of DMN above the background level occurred when a Tenax cartridge was preloaded with DMA. Thus, a blank and DMA preloaded cartridge were used in parallel sampling and compared. Also, in a field experiment air was drawn across a permeation tube containing DMA (~2.5 x 10^{-6} g/min) and into the Tenax cartridge. In different experiments the DMA permeation tube (~2.5 x 10^{-6} g/min) was placed before and after the glass fiber filter used to remove particulates. All experiments were conducted in duplicate. A volume of ~120 ℓ of ambient air was sampled in all cases.

Since urban air often contains substantial concentrations of ozone, a series of laboratory experiments were done to determine whether air containing both NO_x and ozone might be more effective in converting DMA to DMN than air containing only NO_x. Conversion of DMA adsorbed on Tenax and conversion of DMA at low concentrations in air in a glass flow tube were investigated in two additional series of laboratory experiments were conducted. The first focused on the possible conversion of dimethylamine trapped on a Tenax cartridge by polluted air passing through the cartridge. The second was concerned with DMN formation through atmospheric reaction(s) or reactions which might take place on the walls of the sample inlet tube.

The apparatus used to conduct these experiments is shown in Fig. 14. Through the reaction tube a 5 ℓ/min air flow was maintained in all of the experiments performed. Nitric oxide was measured into the stream with a rotometer and a metering valve from a supply tank which contained 54.2 ppm of NO in nitrogen. Ozone was generated by an ultra-violet lamp which had a movable cover so that different concentrations could be obtained. Ozone concentrations >1 ppm were generated with the aid of a Welsbach ozone generator which was inserted into the air-line between the scrubbers and the metering valves (Fig. 14). The concentrations of NO, NO_2, and O_3 were monitored with a Bendix NO_x analyzer and a Bendix Ozone analyzer. The intakes for these instruments were placed at the same point as the intake for the Tenax cartridge sampler through which air was drawn by a Nutech Model 221-A sampler. The sampling cartridge and analyzer inlet tubes were centered in the air flow pattern in the reaction tube. Relative humidity of the air stream was controlled by changing the temperature of the humidifier bath.

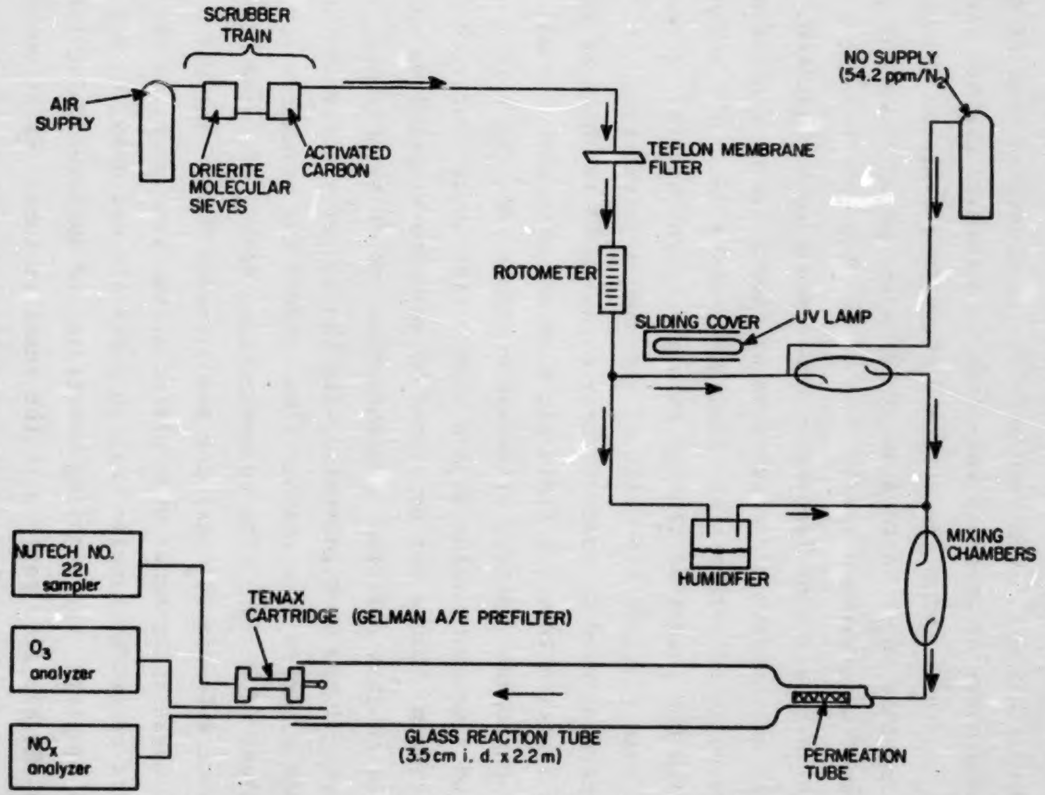

SCRUBBER TRAIN
AIR SUPPLY
DRIERITE MOLECULAR SIEVES
ACTIVATED CARBON
NO SUPPLY (54.2 ppm/N_2)
TEFLON MEMBRANE FILTER
ROTOMETER
SLIDING COVER
UV LAMP
HUMIDIFIER
MIXING CHAMBERS
NUTECH NO. 221 sampler
O_3 analyzer
NO_x analyzer
TENAX CARTRIDGE (GELMAN A/E PREFILTER)
GLASS REACTION TUBE (3.5 cm i. d. x 2.2 m)
PERMEATION TUBE

Figure 14. Schematic of instrumentation and devices for examining in situ formation of N-nitrosodimethylamine on Tenax GC cartridges.

RESULTS AND DISCUSSION

Identification of DMN in Ambient Air

The sampling areas considered in this study are shown in Figures 15-18. Site 1 is the FMC industrial firm, site 2 was a location at the Patapso Sewage Treatment Plant, site 3 at the Chessie Coal Piers, site 4 was DuPont in Belle, WV, site 5 consisted of Union Carbide Corp., Charleston, WV, and site 6 was in Nitro, WV.

Figure 19 depicts the profile of ambient air pollutants in a sample taken during the day in the parking lot area of an industrial site (site 1, Fig. 16). The volume of air collected represents 75 ℓ. A 100 m glass SCOT column containing OV-101 stationary phase was used to effect this separation.

Figure 20 presents a profile of ambient air pollutants in a sample taken during the daylight hours near the Patapsco Sewage Treatment Plant. The sampling apparatus was upwind from the industrial site, but downwind from the Sewage Treatment Plant.

The chromatographic separation of constitutents was also achieved by use of a more polar stationary phase DEGS, coated in a 55 m glass SCOT column, and the results are shown in Fig. 21 (replicate sample of Fig. 19). Semi-polar and polar phases are not well suited to resolution of non-polar (e.g. hydrocarbon) pollutants. However, resolution of semi-polar and polar constituents was significantly better.

Figure 22 shows the mass spectrum of an authentic sample of DMN chromatographed on the 55 m DEGS SCOT column. Figure 22 also depicts a mass spectrum taken at a retention time of 26 min for the ambient air sample collected (Fig. 21) on the industrial site in Baltimore. Comparison of this mass spectrum with that of authentic DMN shows that the two spectra are essentially superimposable and confirms the identification of the unknown as N-nitrosodimethylamine. The lower range (m/e 35) is uncalibrated, so exact correspondence in this range is not observed. The retention time (26 min) of authentic DMN was identical to that of the unknown in Fig. 21. Similar confirmation of the presence of DMN has been obtained for the ambient air profile using OV-225 and OV-101 capillaries (Table 16).

Approximately one month subsequent to the determinations discussed above (November 19-25), the studies were repeated and the presence of DMN

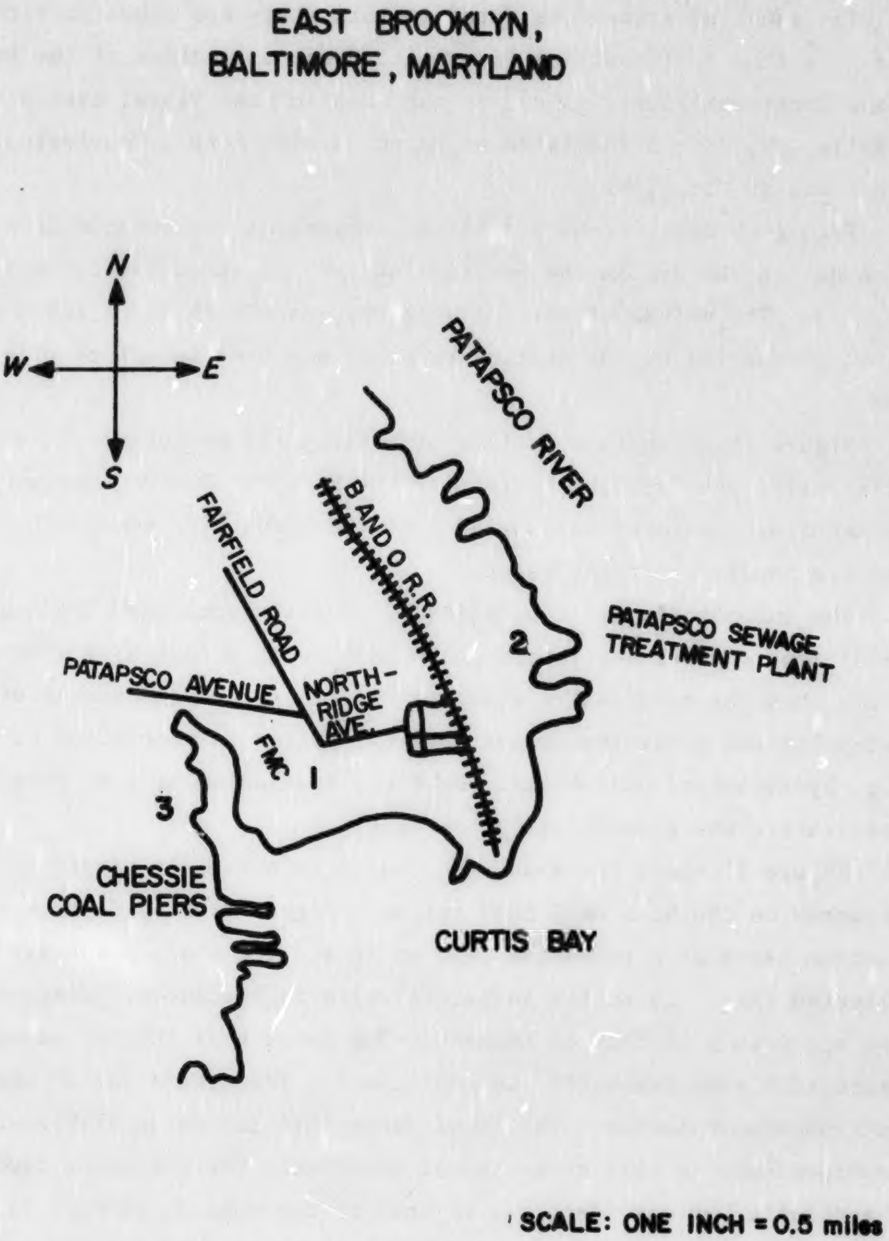

EAST BROOKLYN,
BALTIMORE, MARYLAND
N
W
E
S
PATAPSCO RIVER
B AND O R.R.
FAIRFIELD ROAD
2
PATAPSCO SEWAGE TREATMENT PLANT
PATAPSCO AVENUE
NORTH-RIDGE AVE.
FMC
1
3
CHESSIE COAL PIERS
CURTIS BAY
SCALE: ONE INCH = 0.5 miles

Figure 15. Map of sampling area in East Brooklyn, Baltimore, Maryland

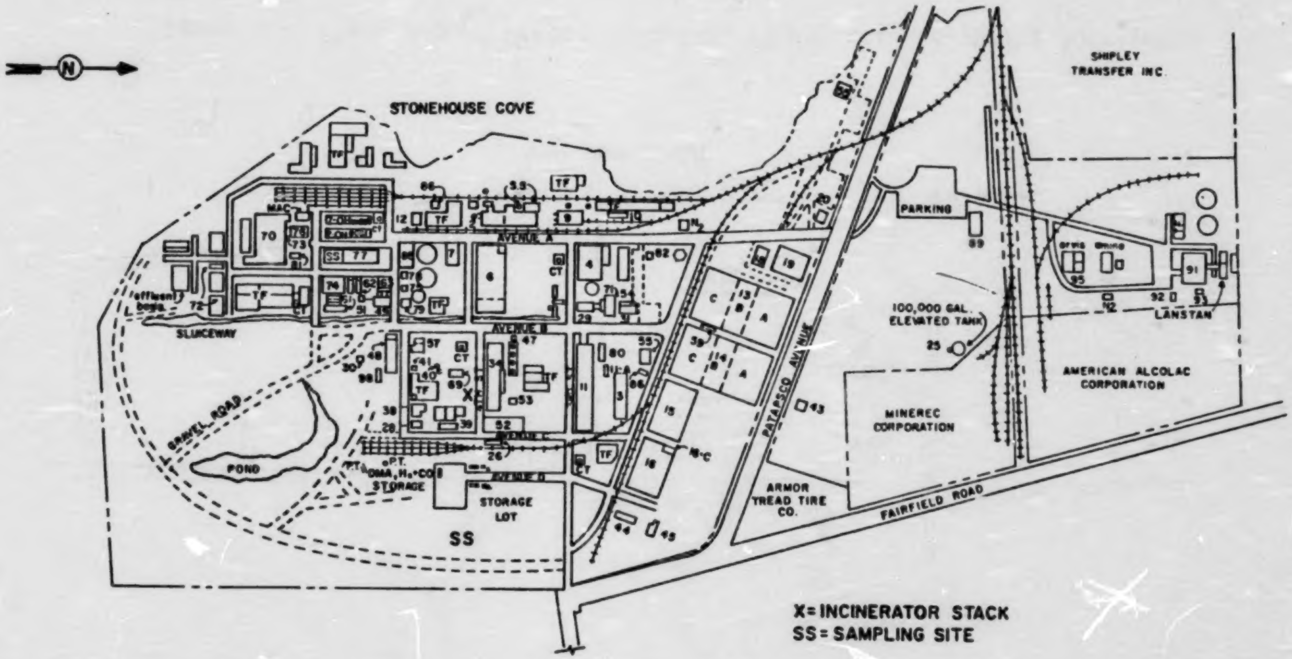

N
STONEHOUSE COVE
SHIPLEY TRANSFER INC.
PARKING
AVENUE A
AVENUE B
SLUICEWAY
GRAVEL ROAD
POND
STORAGE
STORAGE LOT
SS
100,000 GAL. ELEVATED TANK
PATAPSCO AVENUE
MINEREC CORPORATION
AMERICAN ALCOLAC CORPORATION
LANSTAN
ARMOR TREAD TIRE CO.
FAIRFIELD ROAD
X= INCINERATOR STACK
SS= SAMPLING SITE

Figure 16. Plant map of FMC.

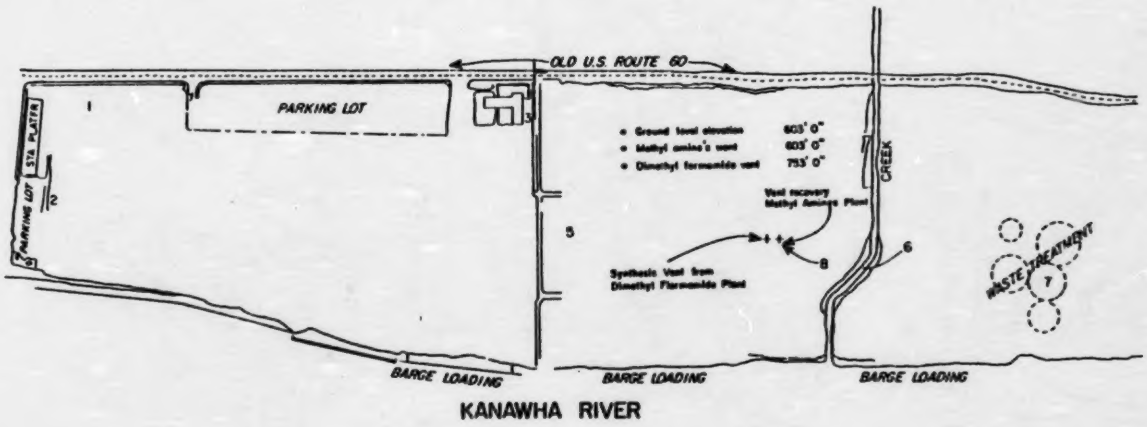

OLD U.S. ROUTE 60
PARKING LOT
STA PLATFR
PARKING LOT
1
2
3
4
5
6
7
8
• Ground level elevation 603' 0"
• Methyl amine's vent 603' 0"
• Dimethyl formamide vent 753' 0"
Vent recovery Methyl Amines Plant
Synthesis Vent from Dimethyl Formamide Plant
CREEK
WASTE TREATMENT
BARGE LOADING
BARGE LOADING
BARGE LOADING
KANAWHA RIVER

Figure 17. Plant map of DuPont in Belle, WV depicting sampling locations.

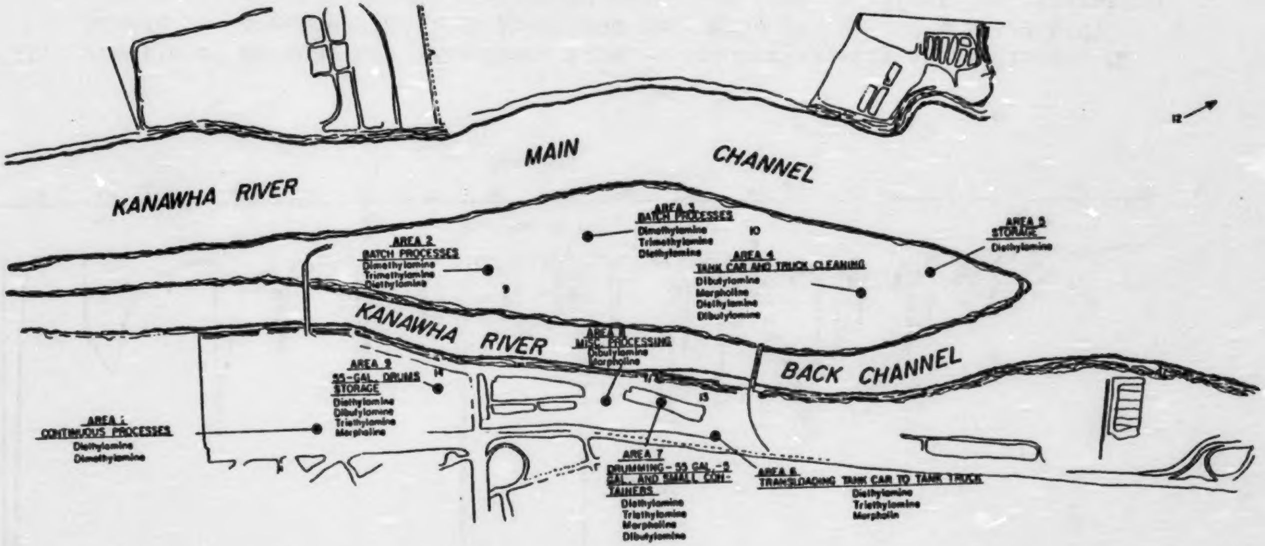

KANAWHA RIVER
MAIN
CHANNEL
KANAWHA RIVER
BACK CHANNEL
AREA 1
CONTINUOUS PROCESSES
Diethylamine
Dimethylamine
AREA 2
BATCH PROCESSES
Dimethylamine
Trimethylamine
Diethylamine
AREA 3
BATCH PROCESSES
Dimethylamine
Trimethylamine
Diethylamine
AREA 4
TANK CAR AND TRUCK CLEANING
Dibutylamine
Morpholine
Diethylamine
Dibutylamine
AREA 5
STORAGE
Diethylamine
AREA 6
TRANSLOADING TANK CAR TO TANK TRUCK
Diethylamine
Triethylamine
Morpholin
AREA 7
DRUMMING - 55 GAL. - 5 GAL. AND SMALL CONTAINERS
Diethylamine
Triethylamine
Morpholine
Dibutylamine
AREA 8
MISC. PROCESSING
Dibutylamine
Morpholine
AREA 9
55-GAL. DRUMS STORAGE
Diethylamine
Dibutylamine
Triethylamine
Morpholine
9
10
13
14
12

Figure 18. Plant map of Union Carbide in South Charleston, WV depicting sampling locations.

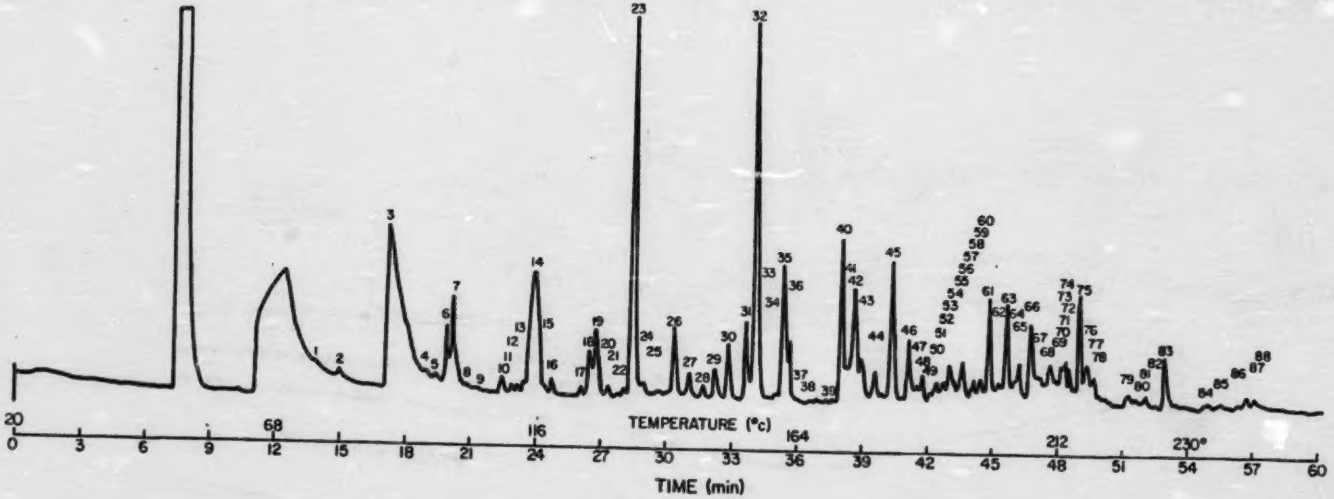


Figure 19. Profile of ambient air pollutants from an industrial site in Baltimore, MD. Sample was taken on 10/14/75 from 3:00 pm - 6:50 pm. A 100 m glass SCOT column coated with OV-101 stationary phase was used to effect the separation: see Table 15 for conditions. Peak No. 27 was established as DMN.

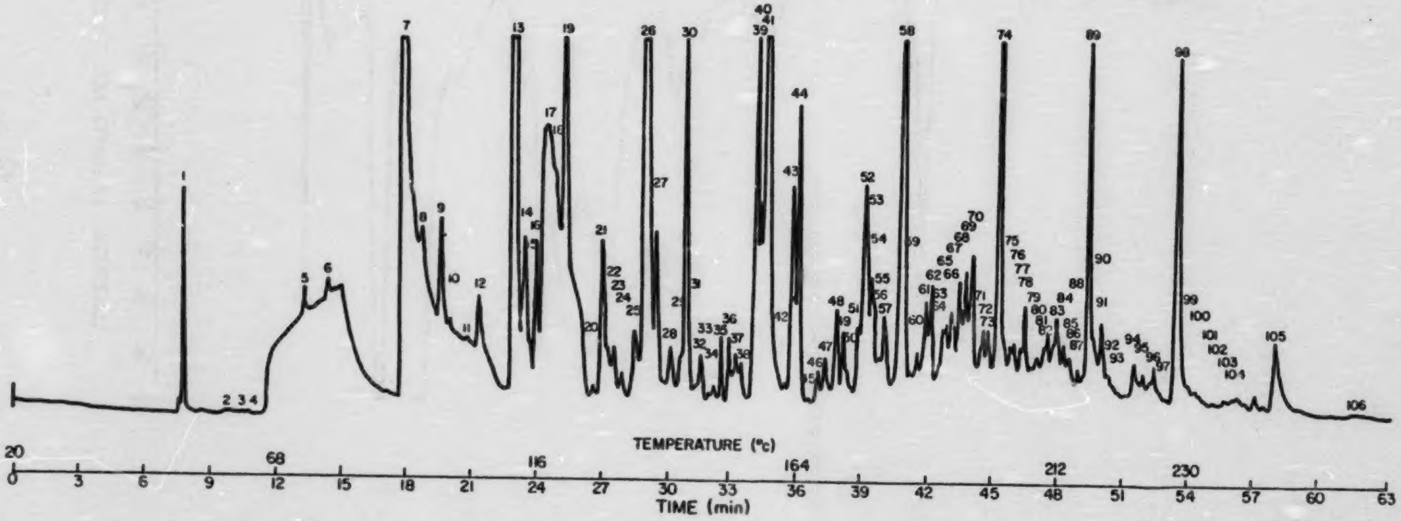


Figure 20. Profile of ambient air pollutants taken on 10/16/75 from 10:00 am - 1:50 pm at the Patapsco Sewage Treatment Plant. Instrumental conditions were identical to Fig. 19.

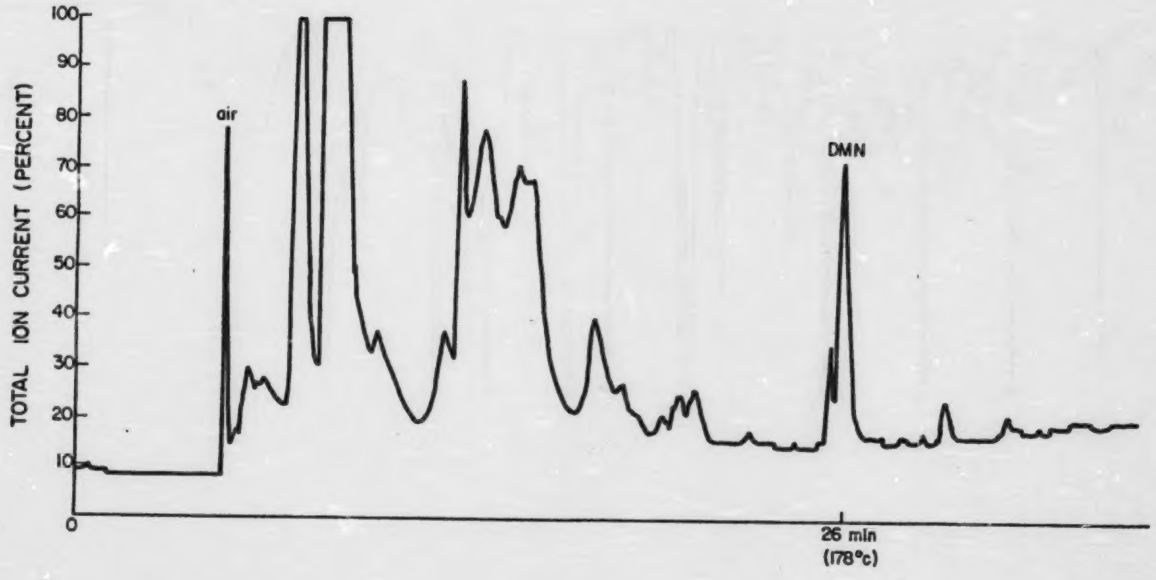
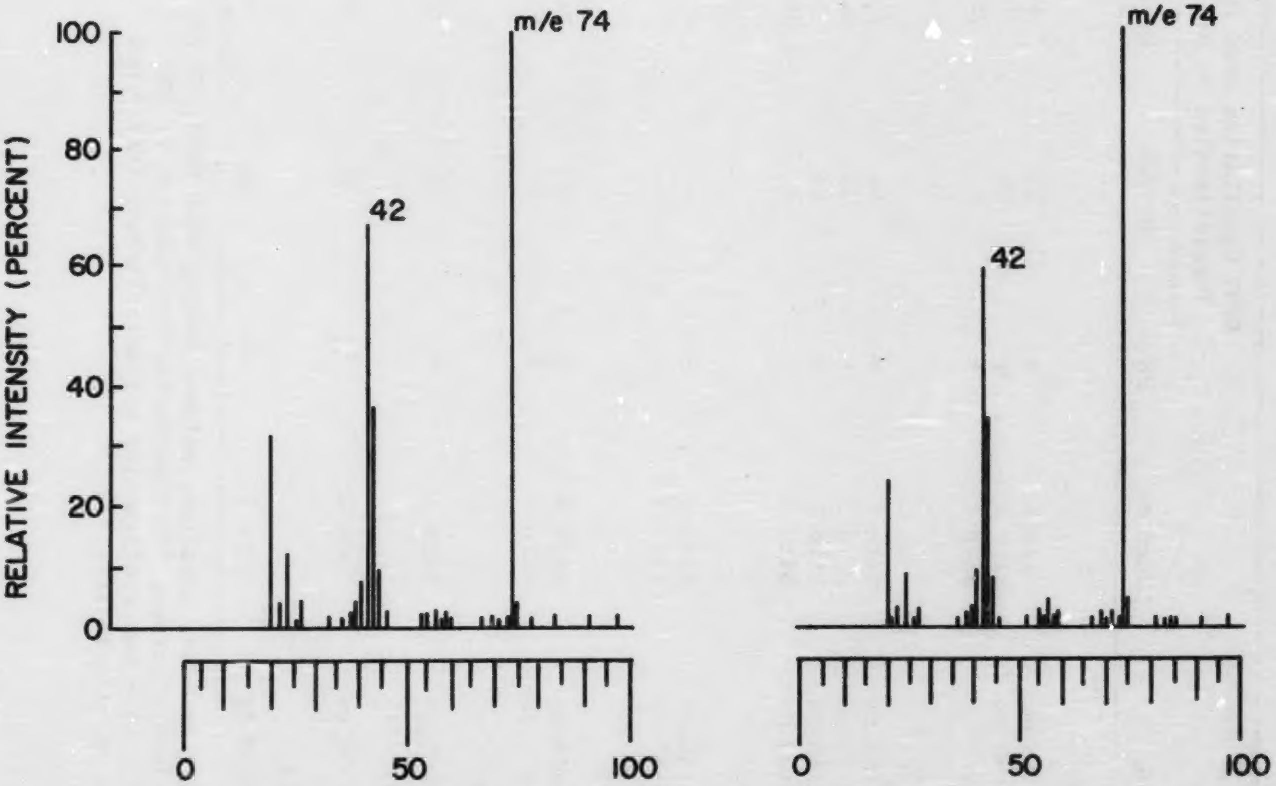


Figure 21. Chromatogram of pollutants from industrial site in Baltimore, Maryland. A replicate sample of that used for Fig. 19. A 55 m DEGS SCOT capillary was used; see Table 15 for operation conditions.



DMN (AUTHENTIC SAMPLE), ANALYZED ON DEGS COLUMN

PEAK AT 26 MIN. IN SAMPLE TAKEN 10/14/75, ANALYZED ON DEGS COLUMN

Figure 22. DEGS Glass SCOT column (55 m) was used in both analyses; 70-205°C at 4°C/min.

Table 16. SAMPLES EXAMINED FOR N-NITROSODIMETHYLAMINE BY GAS LIQUID CHROMATOGRAPHY/MASS SPECTROMETRY/COMPUTER

		SCOT Capillaries used for Identification of DMN[a]		
Date/Time	Location	DEGS	OV-225	OV-101
10/14/75				
11:00 am - 2:50 pm	Site 1	+	NA	+
3:00 pm - 6:50 pm	Site 1	+	NA	+
7:00 pm - 10:50 pm	Site 1	+	+	NA
11/15/75				
11:00 pm - 2:50 pm	Site 1	+	NA	NA
3:00 pm - 6:50 pm	Site 1	+	NA	NA
11:00 am - 2:50 pm	Site 1	+	NA	+
3:00 pm - 6:50 pm	Site 1	+	+	NA
10/16/75				
10:00 am - 1:50 pm	Site 2	-	-	-
2:00 pm - 5:50 pm	Site 2	-	-	-
10/17/75				
9:56 am - 1:46 pm	Site 3	+	NA	NA
2:10 pm - 6:00 pm	Site 3	+	+	NA
11/19/75				
2:00 pm - 4:00 pm	Site 1	+	NA	+
11/24/75				
11:50 pm - 1:50 pm	Site 1	+	NA	+
11/24/75				
6:35 pm - 8:35 PM	Site 1	NA	NA	+

[a] Analysis were on glass capillary columns coated with DEGS, OV-225 or OV-101 stationary phases; (+) = molecular confirmation of DMN established; (-) = DMN confirmation not established; (NA) = not analyzed on this capillary.

was again established (Table 16) in ambient air at the same Baltimore industrial site.

Breakthrough Volumes

Breakthrough volumes for DMN, DMA, NO, NO_2 and H_2O are shown in Table 17. It was evident from these data that the retention volume for DMN was much larger than for the other four substances examined. The breakthrough volumes for NO and NO_2 were extremely small (few ml to zero). This was an important relationship in view of the possibility of in situ reactions occurring on a sorbent bed. The breakthrough volumes (Table 17) indicated that NO, NO_2 and water would not accummulate relative to dimethylamine, thus making the in situ reaction kinetics unfavorable for nitrosation of DMA.

Quantitation of DMN

Since the most intense peak in the mass spectrum was the parent ion (m/e 74, Fig. 23), this ion was selected for quantitating DMN. The selection of m/e 74 proved to be highly specific for DMN when used in combination with a glass capillary coated with DEGS stationary phase and the surfactant benzyl triphenylphosphonium chloride.

Figure 24 depicts a specific ion (m/e 74) chromatogram for an authentic sample of N-nitrosodimethylamine. The retention time of DMN on this capillary was 26 min.

Standard curves for DMN are presented in Figures 25 and 26. Concentrations of DMN ranging from 100 pg - 2,000 ng were prepared on Tenax GC cartridges. Cartridges were desorbed and analyzed by capillary gc/ms with selective ion monitoring. The response of the mass spectrometer was linear over the entire range as shown in Figures 25 and 26. To estimate DMN levels in ambient air, the quantity of DMN on a cartridge was determined and then the concentration in air (ng/m^3) was calculated based on the volume of air sampled.

Concentrations of DMN in ambient air surrounding in industrial site in Baltimore, MD are given in Table 18. Listed are the dates, time periods, and the prevailing meterological conditions during the sampling period. The highest concentration of DMN was 32,000 ng/m^3 (November 19, 2-4:00 p.m.) at the industrial site (1B). At the Chessie Coal Piers (site 3), the highest concentration was ~909 ng/m^3. Upwind from the industrial site, only trace levels of DMN were detected (sewage treatment plant). The recovery of DMN

Table 17. BREAKTHROUGH VOLUMES FOR DMN, DMA, NO, NO_2 AND H_2O[a]

Ambient Temperature (°F)	DMN	DMA	NO	NO_2	H_2O
50	385	60	0.025	0.030	0.060
55	332	55	0.020	0.024	0.055
60	280	50	0.015	0.018	0.050
65	242	45	0.010	0.009	0.045
70	224	40	-[b]	-	0.040
75	204	35	-	-	0.035
80	163	30	-	-	0.030
85	156	25	-	-	0.025
90	127	15	-	-	0.020
100	107	10	-	-	0.015
105	93	5	-	-	0.005
110	79	1	-	-	-

[a] Breakthrough volume expressed as ℓ/2.2 g of Tenax GC (35/60 mesh) in a sampling cartridge.

[b] The breakthrough volume was not distinguishable from the sweep volume of the carrier gas.

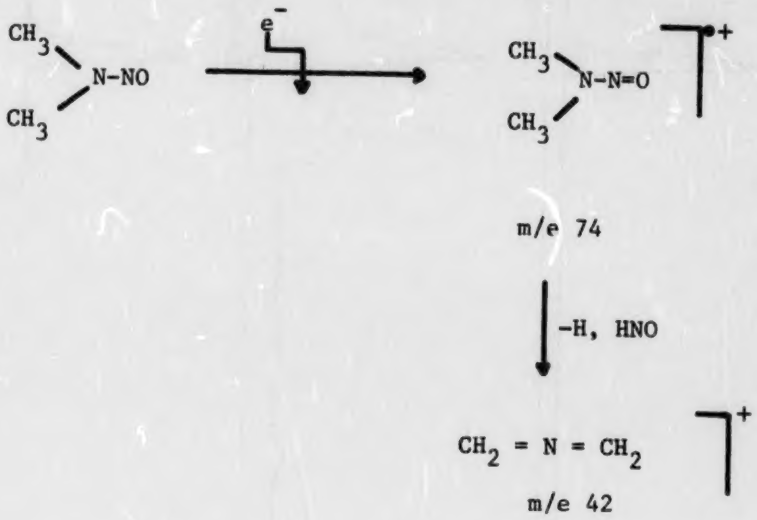

e⁻
m/e 74
-H, HNO
m/e 42

Figure 23. Mass cracking pattern for N-nitrosodimethylamine

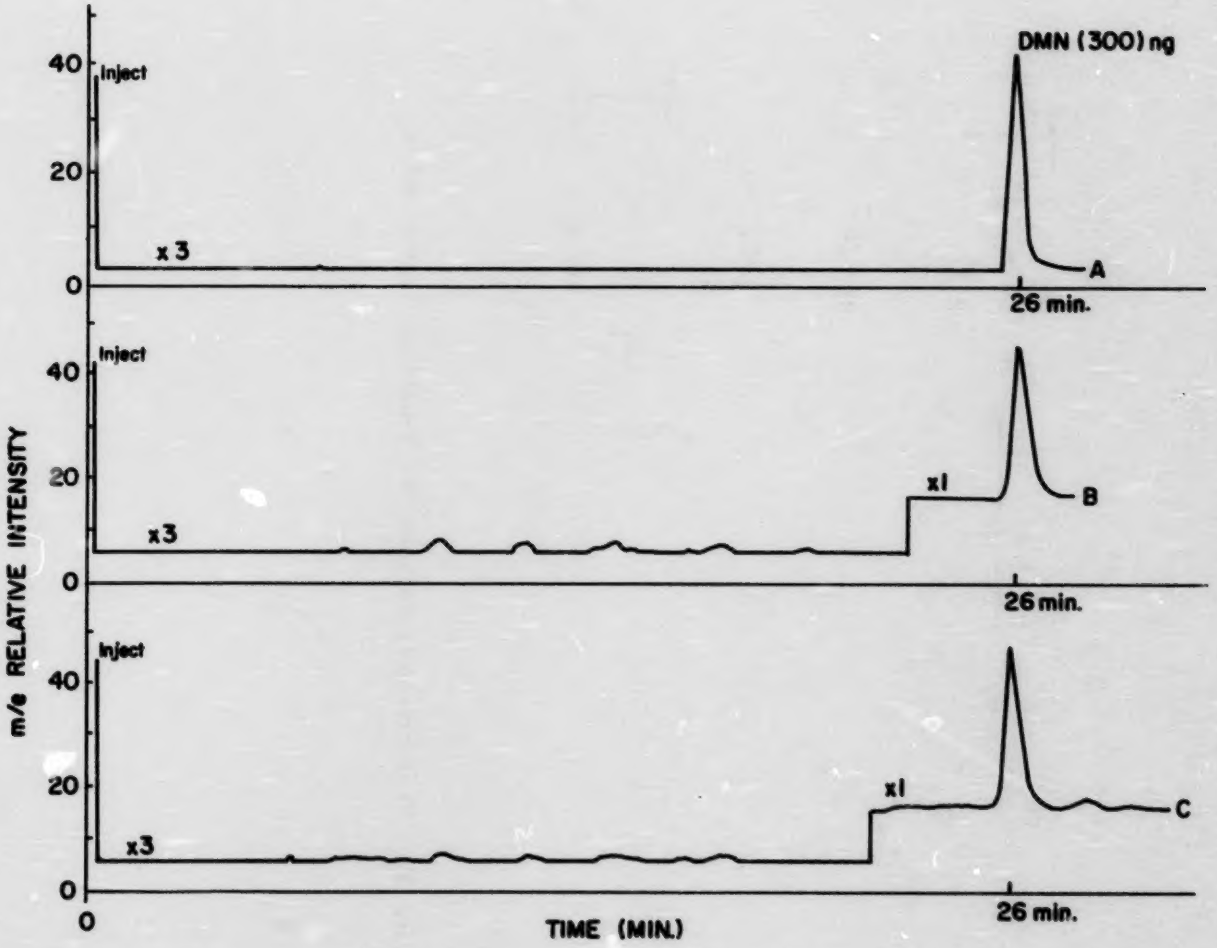


Figure 24. Single ion (m/e 74) chromatogram for N-nitrosodimethylamine. A, B, C, are traces for standard DMN, and replicate field samples, respectively. Analysis on DEGS column, standard conditions.

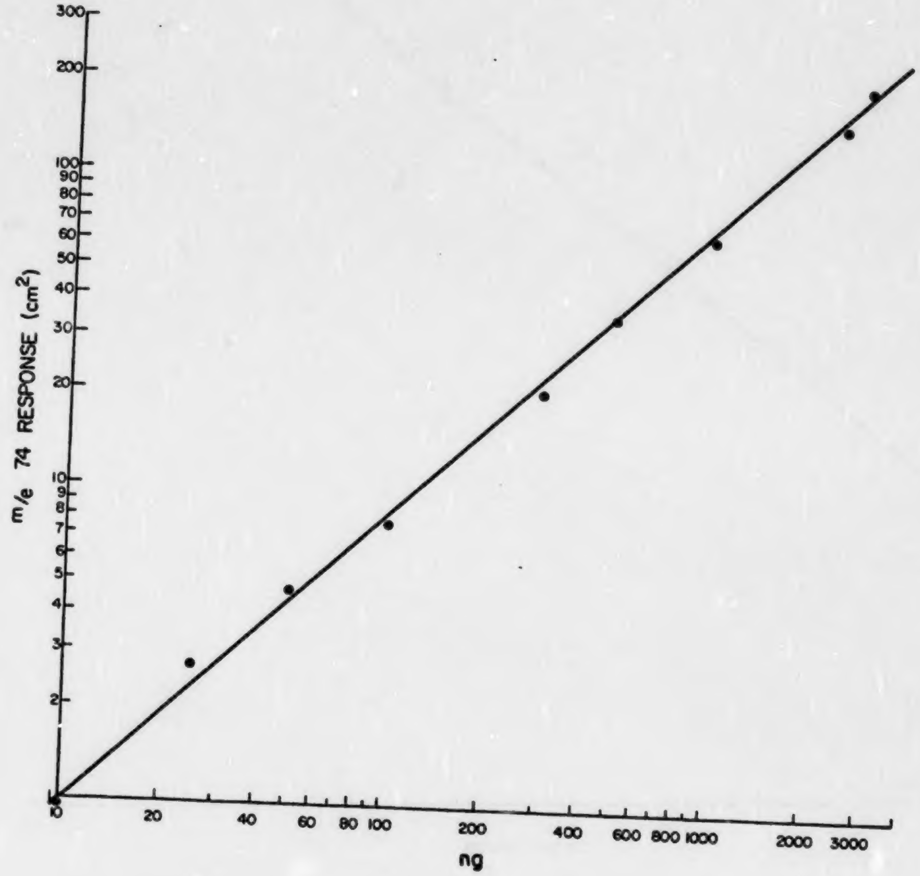


Figure 25. Standard curve for N-nitrosodimethylamine.

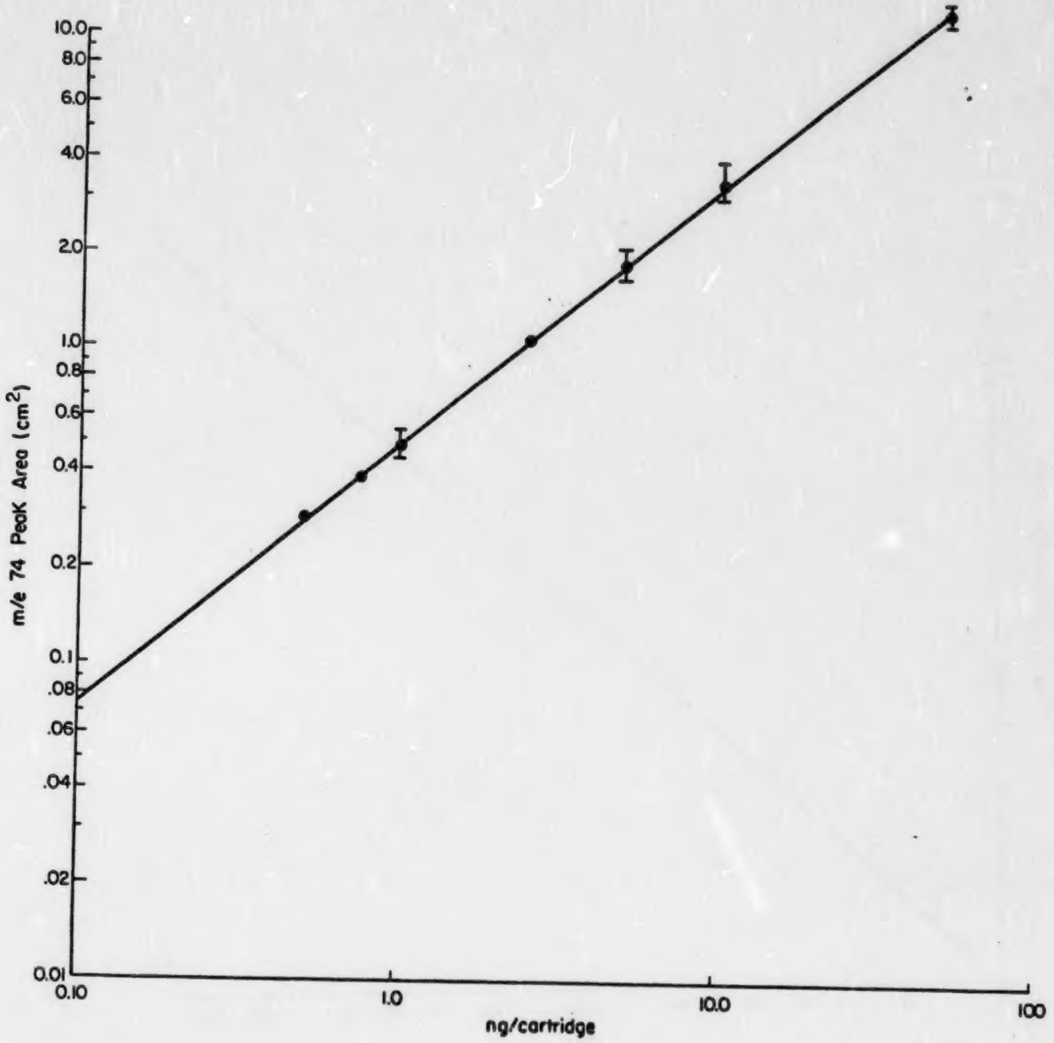


Figure 26. Standard curve for N-nitrosodimethylamine.

Table 18. SAMPLING CONDITIONS AND CONCENTRATIONS OF N-NITROSODIMETHYLAMINE IN AMBIENT AIR

Date	Time (EDT)	Site[a]	Temperature (°F)	Relative Humidity (%)	Wind Direction	Wind Speed (KTS)	DMN ng/m^3
10/14/75	11:00 am - 2:50 pm	1a	83	40-50	WNW	10	2,133
	3:00 pm - 6:50 pm	1a	85	45-50	WNW	7	10,500 ± 1,167
	7:00 pm - 10:50 pm	1a	74	65-85	WSW	7	1,375 ± 125
	11:00 pm - 2:50 am	1a	65	90-97	calm	-	416
10/15/75	3:00 pm - 6:50 am	1a	61	97	S	3	517
	11:00 am - 2:50 pm	1a	85	40-50	WSW	8-10	3,200
	3:00 pm - 6:50 pm	1a	83	40-50	WSW	5-8	13,437 ± 937
10/16/75	10:00 am - 1:50 pm	2	72	45-57	NNW	9-11	<0.6
	2:00 pm - 5:50 pm	2	72	45-50	NNW	5-12	<0.6
10/17/75	9:56 am - 1:46 pm	3	55	88-94	ENE	7-9	909
	2:10 pm - 6:00 pm	3	55	94-100	E	10-14	84
11/19/75	2:00 pm - 4:00 pm	1b	65	56	E	3	32,000 ± 1,500
11/20/75	3:45 pm - 5:45 pm	1c	68	57-73	SW-S	3-6	1,950
	8:20 pm - 10:20 pm	1d	57	71	S-SW	4	1,360 ± 510

(continued)

Table 18 (cont'd)

Date	Time (EDT)	Site[a]	Temperature (°F)	Relative Humidity (%)	Wind		DMN ng/m^3
					Direction	Speed (KTS)	
11/24/75[b]	11:50 am - 1:50 pm	1e	62	72	NW	3	20,000 ± 4,000
	1:55 pm - 3:55 pm	1e	64	74	NNW	4	14,000 ± 200
	6:35 pm - 8:35 pm	1e	59		NNW	3	26,000 ± 500
11/25/75	1:48 pm - 3:48 pm	1f	65	68	-	4	7,600

[a] Sites were shown on Figure 1, letters indicate locations on the site.

[b] Replicate cartridges were sampled in parallel except one for each time period was used to examine potential *in situ* reactions; see text for details.

from sampling cartridges which were transported to and from the field was >95%.

Figure 24 also depicts single ion chromatograms for DMN for duplicate sampling cartridges which were taken on October 14. The reproducibility of the entire quantitation method was approximately ±10%, as exemplified by replicate determinations (Table 18).

The detection limit observed for the m/e 74 ion was approximately 0.2 parts-per-trillion when the ambient air temperature during field sampling was 50°F. Thus the minimum amount of DMN which can be quantitated under these field sampling conditions was approximately 2 parts-per-trillion.

Single ion plots for N-nitrosodimethylamine of samples taken from DuPont and Union Carbide are shown in Figures 27 and 28. In separate experiments, the retention time for N,N-dimethylformamide was determined in order to assess whether the monitoring of m/e 74 ion for DMN would be contamined by this compound. Although N,N-dimethylformamide has a molecular ion of 73, if present in large quantities it is conceivable that the intensity of the ^{13}C isotope would increase until the 74 ion intensity would become significant. The retention time for N,N-dimethylformamide was determined to be 2 min longer than that of DMN on the SCOT glass capillary. Therefore, this compound does not interfere with the quantitation of DMN. No other interferences are known to occur with an identical retention time (27.2 min, Fig. 27 and 28) of DMN as well as an m/e 74 ion.

Using the above described techniques, the concentration of DMN in ambient air was determined in the plant area of DuPont and Union Carbide. Table 19 depicts these results. On December 1, the highest concentration of DMN was observed as location No. 4 (38 ng/m^3). During the early morning hours of December 2, it reached a level of 68.5 ng/m^3. During the sampling period on the evening of December 2 to 3:00 AM, the concentration of DMN observed on the Union Carbide was extremely low or non-detectable. The highest concentration of DMN was 40 ng/m^3 at location 13 on December 13. On December 4, further sampling was conducted on the DuPont property at locations 5, 6, 7 and 8. The highest levels of DMN observed for the entire week occured at location 6 (980 ng/m^3). These locations were along and near an aeration system and waste treatment area. The temperature of the water at

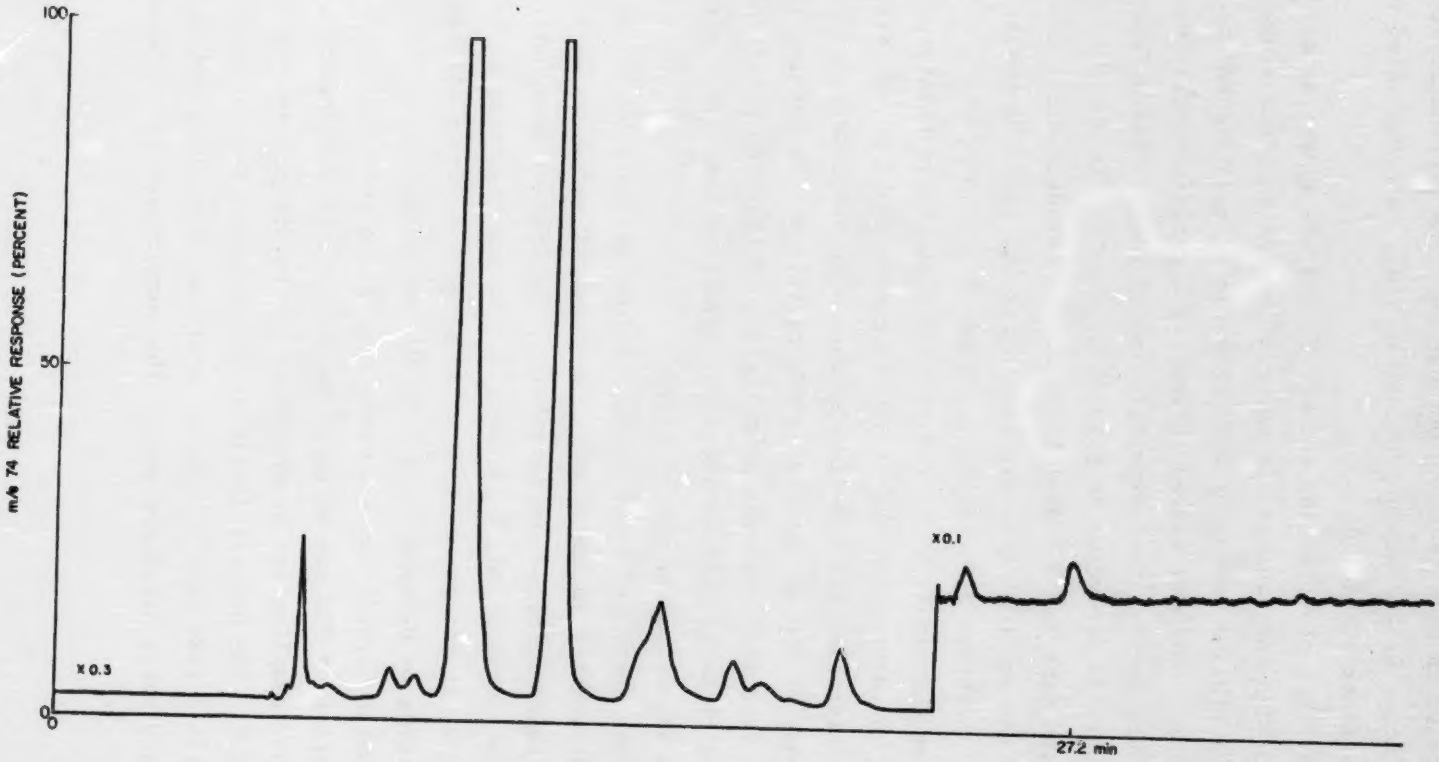


Figure 27. Single ion (m/e 74) current profile of ambient air sample taken at locations No. 2 on DuPont property in Belle, WV.

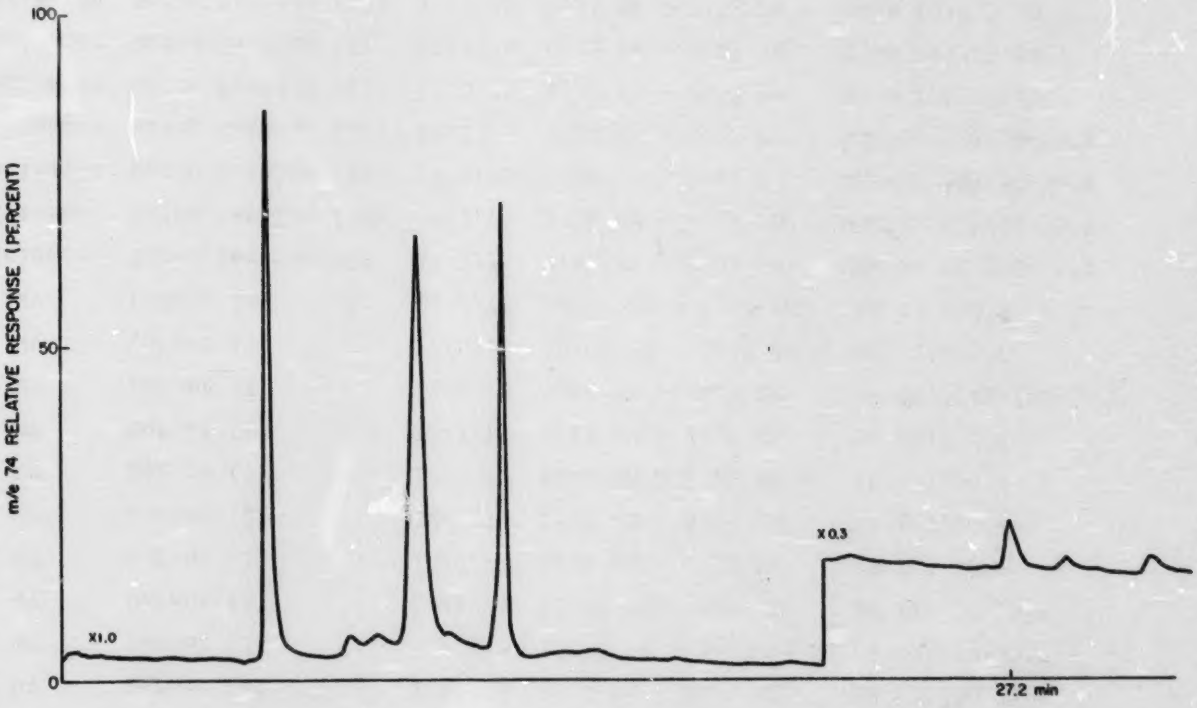


Figure 28. Single ion (m/e 74) current profile of ambient air sample taken at location No. 13 on Union Carbide property in South Charleston, WV.

Table 19. SAMPLING CONDITIONS AND CONCENTRATIONS OF N-NITROSODIMETHYLAMINE IN AMBIENT AIR IN THE KANAWHA VALLEY, WV

Site	Location	Date	Time	Wind (Knots)/Temperature	ng/m^3
Belle, WV	DuPont (1)[a]	12/1/75	9:30 PM - 2:17 AM	NW (2)/30-35°F	10.1
Belle, WV	DuPont (2)	12/1/75	9:24 PM - 2:19 AM	NW (2)/30-35°F	4.2
Belle, WV	DuPont (3)	12/1/75	10:16 PM - 3:09 AM	NW (2)/30-35°F	3.9
Belle, WV	DuPont (4)	12/1/75	10:07 PM - 3:97 AM	NW (2)/30-35°F	38.0 ± 6
Belle, WV	DuPont (1)	12/2/75	2:29 AM - 6:52 AM	SE (4)/30°F	26.0 ± 4
Belle, WV	DuPont (2)	12/2/75	2:28 AM - 6:53 AM	SE (4)/30°F	12.9 ± 2[c]
Belle, WV	DuPont (3)	12/2/75	4:00 AM - 7:11 AM	SE (4)/30°F	67.0
Belle, WV	DuPont (4)	12/2/75	3:17 AM - 7:12 AM	SE (4)/30°F	68.5 ± 5
Belle, WV	DuPont (2)	12/2/75	9:00 PM - 3:02 AM	SE (2)-calm/40-50°F	59
Belle, WV	DuPont (3)	12/2/75	10:02 PM - 3:18 AM	SE (2)/40°F	77.6 ± 6
Belle, WV	DuPont (4)	12/2/75	10:05 PM - 3:00 AM	SE (2)/40°F	103.0
S. Charleston	Union Carbide (9)	12/3/75	2:41 PM - 6:01 PM	WNW→NW (2)/50-55°F	<1
S. Charleston	Union Carbide (10)	12/3/75	3:12 PM - 5:12 PM	WNW→NW (2)/50-55°F	ND[b]
S. Charleston	Union Carbide (11)	12/3/75	3:36 PM - 6:27 PM	WNW→NW (2)/50-55°F	13.6
S. Charleston	Union Carbide (12)	12/3/75	3:38 PM - 5:28 PM	WNW→NW (2)/50-55°F	11.6
S. Charleston	Union Carbide (11)	12/3/75	6:33 PM - 8:53 PM	NW→N (2)/45-50°F	ND
S. Charleston	Union Carbide (9)	12/3/75	6:16 PM - 8:19 PM	NW→N (2)/45-50°F	<1
S. Charleston	Union Carbide (13)	12/3/75	5:51 PM - 7:56 PM	NW→N (2)/45-50°F	ND[c]
S. Charleston	Union Carbide (14)	12/3/75	6:15 PM - 8:40 PM	NW→N (3)/45-50°F	ND

(continued)

Table 19 (cont'd)

Site	Location	Date	Time	Wind (Knots)/Temperature	ng/m^3
S. Charleston	Union Carbide (11)	12/3/75	6:33 PM - 8:43 PM	NW→N (3)/45-50°F	56
S. Charleston	Union Carbide (11)	12/3/75	8:28 PM - 10:30 PM	N→NNE (3)/40-45°F	ND
S. Charleston	Union Carbide (13)	12/3/75	8:03 PM - 10:17 PM	N→NNE (3)/40-45°F	40 ± 2
S. Charleston	Union Carbide (14)	12/3/75	8:47 PM - 10:44 PM	N→NNE (3)/40-45°F	ND
Belle, WV	DuPont (5)	12/4/75	5:10 PM - 7:11 PM	NE (2)-calm/54-60°F	ND
Belle, WV	DuPont (6)	12/4/75	3:26 PM - 5:24 PM	NE (2)-calm/60°F	980
Belle, WV	DuPont (7)	12/4/75	4:00 PM - 6:05 PM	calm (plumes/60°F straight up)	500
Belle, WV	DuPont (8)	12/4/75	7:06 PM - 9:06 PM	NE (2)-calm/60°F	576
Nitro, WV	I-60 & WV25	12/5/75	11:58 AM - 3:48 PM	SW (10)/65°F	ND
Nitro, WV	I-60 & WV25	12/5/75	11:59 AM - 3:49 PM	SW (10)/64°F	ND

[a] See industrial plant map for precise location.

[b] ND = not detected.

[c] Part of Artifact Experiment.

the aeration system was ~110°F. The sampler was located near this point for a period of 2 hr (location 6).

DMN was not detected on December 5 when sampling was conducted in Nitro, WV near the corner of Interstate 60 & WV 25.

In Situ Formation of DMN

An important species for nitrosation is nitrous acid and since a small retention volume for water was observed, it was conceivable that some of the NO_x could have been converted to nitrous acid ($NO + NO_2 + H_2O \rightleftharpoons 2HONO$). In light of this possibility we examined the yield of DMN under a series of various laboratory and field sampling conditions. Table 20 depicts the yield of DMN from potential in situ reactions on Tenax GC during sampling in the presence of DMA, NO, NO_2 and/or water. Cartridges were prepared by drawing through them 50 ℓ of air containing 5 ppm of DMA. Then an additional 15 ℓ of air containing 1, 10 or 250 ppm of NO were sampled. No DMN was detected. Also, when 50 ℓ of air containing 4.5 ppm DMA were passed through a cartridge and then equal molar quantities of NO and NO_2 (expt. 5) were sparged into an air stream entering the cartridge at a relative humidity of 75%, no DMN was detected. When the concentration of NO was increased to 1 ppm, ~10 ppt of DMN was observed. At a concentration of 10 ppm of NO (75% relative humidity), the yield of DMN reached ~300 ppt. Storing cartridges at -20°C for a period of 2 weeks gave similar results as those which were analyzed immediately after the in situ reaction experiment had been completed (Table 20 expts. 10-13). These data show that at high concentrations of NO_2 it was possible to produce DMN; however, it is generally recognized that the concentrations of NO_x in ambient air rarely exceed 1 ppm. Thus, under these circumstances the quantitation of DMN was possibly down to a level of 10 ppt without an appreciable contribution from in situ reactions.

In situ enhancement of DMN collection was not detected when dimethylamine was introduced into the air sampling stream (Table 18, 11/24/75). Analysis of cartridges which were sampled in parallel fashion (one was a reference blank) indicated that the concentrations were within the experimental reproducibility of the technique. It was concluded from these experiments that any formation of DMN from an in situ reaction between dimethylamine and NO_x was negligible and that the DMN measured in ambient air was

Table 20. YIELD OF DMN FROM IN SITU REACTION(s) ON TENAX GC CARTRIDGES DURING SAMPLING IN THE PRESENCE OF DMA, NO, NO_2 AND H_2O

Experiment No.[a]	Concentration Sampled (ppb)			H_2O (%RH)[b]	DMN Yield (ppt)
	DMA	NO	NO_2		
1	5,000	1	-	72	ND[c]
2	5,000	10	-	72	ND
3	5,000	250	-	72	ND
4	4,500	-	-	72	ND
5	4,500	500	500	75	ND
6	4,500	1,000	-	75	10
7	4,500	1,000	1,000	75	15
8	4,500	5,000	-	75	35
9	4,500	10,000	-	75	~300
10	5,000	1	-	72	ND
11	5,000	10	-	72	ND
12	5,000	250	-	72	ND
13	4,500	1,000	-	75	15

[a] See text for explanation of experimental design; experiments 10-13 were duplicates of 1-3 and 6 except cartridges were stored for 2 week at -20°C.

[b] Percent relative humidity at 26°C.

[c] Detection limit was ca. 0.3 ppt.

originating from a point source. The industrial site was known to produce DMN as an intermediate in a synthetic process.

Field experiments were also conducted at the Union Carbide and DuPont sampling sites in order to either support or refute the possibility of an *in situ* reaction. The rationale was to demonstrate whether an enhancement in the quantity of DMN occurred during sampling since the preloaded dimethylamine would become exposed to ambient levels of NO_x. Two sets of cartridges were utilized for this artifact experiment at the DuPont (location 2) and Union Carbide (location 13) properties. In both cases we did not observe an increase in the background level of DMN which was detected and quantitated by monitoring m/e 74 ion.

Additional laboratory experiments were conducted whereby Tenax GC cartridges (1.5 cm x 6.0 cm) were preloaded with dimethylamine (DMA) by passing through them nitrogen gas which contained a known quantity of DMA from a calibrated permeation tube ($^1H_6$-DMA or $^2H_6$-DMA). Each of these cartridges was used to sample a 10 liter volume of air containing known levels of NO, NO_2, O_3, and water. Then the cartridges were thermally desorbed and analyzed for $^1H_6$-DMN or $^2H_6$-DMN. The results are summaried in Table 21. One cartridge, preloaded with $^2H_6$-DMA was submitted for gc/ms analysis (m/e 80) without further processing to determine the level of $^2H_6$-DMN present in the amine as a contaminant (Experiment No. 1). No $^2H_6$-DMN was found in this sample. Samples of air containing 500 ppb NO were taken at 50% and 90% relative humidity, also without producing any $^2H_6$-DMN was formed. Four experiments (Nos. 5-8) were run in which air with ~300 ppb NO and ~200 ppb NO_2 was sampled. Two of these (Nos. 7 & 8) were run with low humidity air. In two cases (Nos. 6 & 8) a very small volume of nitrogen was used to preload the $^2H_6$-DMA so that it would be confined to a relatively narrow zone in the cartridge bed. In the other two cases (Nos. 5 & 7) a 10 liter volume of nitrogen was used to preload the $^2H_6$-DMA so that it was distributed in a much broader zone in the sorbent bed. The amounts of $^2H_6$-DMN formed did not fall into any definite pattern. Except for Experiment No. 8 they are about the same as the amount formed in Experiment No. 4. The amount of ozone added to the air stream was increased so that most of the NO was converted to NO_2 leaving small residual amounts of NO and ozone (Nos. 9-12). This resulted in formation of increased quantities of

Table 21. EFFECT OF OZONE, NO, NO_2 AND DMA ON IN SITU FORMATION OF DMN

Experiment No.	O_3 added (ppb)	O_3 excess (ppb)	NO_x (ppb)	NO (ppb)	NO_2 (ppb)	T°C	%RH	DMA (nM)/(liters)	DMN (nM)	% yield
1	0	0	0	0	0	25	-	202/10	0	0
2	0	0	500	500	0	25	50	202/10	0	0
3	0	0	500	500	0	25	90	202/0.151	0	0
4	80	0	500	420	80	25	50	202/10	0.18	0.089
5	200	0	500	300	200	25	50	202/10	0.32	0.158
6	200	0	510	310	200	24	67	202/0.151	0.14	0.069
7	210	0	490	280	210	27	10	202/10	0.12	0.059
8	210	0	530	320	210	27	10	202/0.151	0.65	0.322
9	510	10	530	30	500	25	50	202/10	0.54	0.267
10	479	9	515	45	470	26	90	202/0.151	0.92	0.455
11	550	50	540	40	500	26	10	202/10	0.12	0.059
12	489	9	520	40	480	27	10	202/0.151	1.46	0.723
13	650	150	500	0	500	26	50	202/10	0.86	0.426
14	640	140	500	0	500	27	90	202/0.151	1.24	0.614
15	650	150	500	0	500	26	10	202/10	0.93	0.460
16	640	140	500	0	500	27	10	202/0.151	1.46	0.723
17	482	2	540	60	480	24	50	404/0.42	0.58	0.144
18	680	180	500	0	500	24	50	404/0.42	0.25	0.062

(continued)

Table 21 (cont'd)

Experiment No.	O_3 added (ppb)	O_3 excess (ppb)	NO_x (ppb)	NO (ppb)	NO_2 (ppb)	T°C	%RH	DMA (nM)/liters)	DMN (nM)	% yield
19	~1500	~1000	500	0	500	26	50	202/0.215	2.78	1.376
20	~2500	~500	~2000	0	~2000	26	50	202/0.215	1.16	0.574
21	~3000	~1000	~2000	0	~2000	26	50	202/0.215	1.04	0.515

$^2H_6$-DMN in three of the experiments. More $^2H_6$-DMN was formed on the cartridges which had been loaded with $^2H_6$-DMN concentrated in a small volume of nitrogen (Nos. 10 & 12) than was formed on cartridges loaded with the same amount of $^2H_6$-DMA in a large volume of nitrogen (Nos. 9 & 11). The ozone was further increased so that there was no substantial excess of it at the end of the flow tube and all of the NO was converted to NO_2 (Nos. 13-16). Again, the amount of $^2H_6$-DMN produced was generally larger and more was produced on the cartridges which were loaded with concentrated zones of $^2H_6$-DMA (Nos. 14 & 16). Doubling the amount of $^2H_6$-DMA on the cartridge did not result in any increase in the amount of $^2H_6$-DMN formed (Nos. 17 & 18). It was apparent that a high concentration of DMA in a small volume of sorbent bed would produce more DMN than the same amount of DMA distributed evenly through the entire bed.

There was no clear indication that the level of relative humidity had any significant effect on the results. This was not surprising in view of the very large excess of water over the concentrations of other potential reactants at even the lowest levels of relative humidity. A constant, convenient level of 50% relative humdity was adopted for further experiments.

The concentrations of NO_x and ozone in these experiments were at levels approximating the highest found in polluted air. In order to test the possible effects of conditions that might prevail at extremely elevated levels of NO_x in plumes coming from a point source, three experiments (Nos. 19-21) were conducted at much higher NO_x and ozone concentrations. There was a substantial increase in the amount of DMN formed when the ozone level was increased (No. 19), but no indication of any increase from higher levels of NO_2 (Nos. 21 & 21).

The principal result of this series of experiments is that under extreme conditions of NO_2 and ozone pollution in the conversion of 202 nM of DMA on a Tenax cartridge was small (Less than 1%). However it must be remembered that the breakthrough volumes of DMA was not exceeded in these experiments. Furthermore, the breakthrough volume of DMN is much larger than that of DMA. If a volume of polluted air larger than the breakthrough volume of DMA had passed through the cartridge, presumably even more of the DMA would have been converted, and the resulting DMN would have been retained on the cartridge. Thus it would be misleading to attempt to extrapolate these results to higher sample volumes. On the otherhand, the concentrations of DMA used to load the cartridges (0.5-33 ppm) were quite large, approximating the levels that could be found in ambient air in the immediate vicinity of a primary source. The results of this study suggest that the efficiency of conversion of DMA to DMN would be greatly dependent on the concentration of DMA in the sorbent bed. This means that more DMN would be formed on the cartridge if the DMA concentration fluctuated during the sampling period than if the same amount of DMA were drawn into the cartridge at a constant, low concentration.

The presence of NO_2 was clearly necessary for formation of DMN. This suggests that the mechanism was formation of nitrous acid from NO, NO_2 and water with subsequent reaction between nitrous acid and DMA to form DMN. The smaller yields of DMN in Experiment Nos. 17, 18, 20 and 21 in which extremely high reactants levels were used were surprising. It would be interesting to know the reactant concentrations at which DMN formation would reach a maximum.

A permeation tube containing $^2H_6$-DMA was placed in the upstream end of the reaction tube (Fig. 14) so that the air passing down the tube would carry with it a very low level of $^2H_6$-DMA. Various concentrations of NO, NO_2 and ozone were introduced into the air stream and samples of NO_2, ozone and organic vapors were taken at the downstream end of the reaction tube. The results are summarized in Table 22. In one experiment (No. 22) neither NO nor ozone was added to the air, and no $^2H_6$-DMN was produced. Air containing 500 ppb NO without ozone was passed through the tube, and again no $^2H_6$-DMN was found (No. 23). However, substantial quantities of $^2H_6$-DMN, somewhat larger than those formed in the comparable in situ experiments, were found when ozone was added to the air stream (Nos. 24-26). These experiments were conducted with the reaction tube covered with aluminum foil. In order to test the effect of ultra-violet radiation on formation of DMN in the flow tube, a 22 cm length near the upstream end was uncovered and irradiated with a Sylvania 110V, 275W sunlamp (Nos. 27-30). The flow tube was constructed of 40 mm O.D. standard wall (~2 mm) Pyrex® tubing. Light penetrates this thickness of Pyrex with 50% transmission at $\lambda = 3170\text{Å}$ (1). Oxygen and NO photolyses occur only at lower wavelengths

Table 22. FORMATION OF DMN FROM OZONE, NO, NO_2 AND DMN IN A FLOW TUBE

Experiment No.	O_3 added (ppb)	O_3 excess (ppb)	NO_x (ppb)	NO (ppb)	NO_2 (ppb)	T°C	%RH	$^1H_6$-DMA (nM)/(liters)	$^2H_6$-DMA (nM)/(liters)	DMN (nM)	DMN-d_6 (nM)	% yield
22	0	–	0	0	0	25	50	–	202/15.6	–	0	0
23	0	–	500	500	0	24	50	–	202/15.6	–	0	0
24	190	0	500	340	190	24	50	–	202/15.6	–	0	0
25	487	7	520	40	480	25	50	–	202/15.6	–	1.14	0.564
26	680	180	500	0	500	25	50	–	202/15.6	–	~3.78	1.871
27[a]	0	–	500	500	0	26	50	–	202/15.6	–	1.93	0.955
28[a]	220	0	510	290	220	27	50	–	202/15.6	–	0.140	0.069
29[a]	475	15	510	50	460	26	50	–	202/15.6	–	0.6	0.297
30[a]	680	180	500	0	500	26	50	–	202/15.6	–	1.82	0.901
31[b]	210	0	530	320	210	26	50	–	202/15.6	–	0.34	0.168
											0.22	0.109
												Ratio: (Formed in Tube): (Formed on Cartridge)
32	690	190	500	0	500	26	50	392/0.422[c]	~388/30	2.67	8.63	3.23
33	690	190	500	0	500	26	50	392/0.422[c]	~420/32.5	2.67	8.24	3.09
34	690	190	500	0	500	26	50	392/0.422[c]	~388/30	2.44	7.06	2.89
35	700	200	500	0	500	22	50	~140/30	140/0.125[c]	lost	lost	
36	700	200	500	0	500	22	50	~140/30	140/0.125[c]	4.44	1.96	2.27

[a] Irradiated with UV lamp, 22 cm zone centered 1.7M from downstream end of tube.

[b] Irradiation zone centered 0.6 cm from downstream end of tube.

[c] Preloaded on cartridge.

than could have penetrated the tube, but NO_2 and O_3 are photolyzed to produce oxygen atoms under these conditions, so that formation of DMN by a free radical mechanism might be possible. However some $^{2}H_{6}$-DMN was found even in the absence of added ozone. It could have formed in a photochemical reaction, but it is more likely DMN formed in previous runs was stripped from the walls of the tube as a result of its being heated by the lamp (see below). Regardless whether DMN is formed by a second (photochemical) mechanism, it appears significant that in general less of it was found when part of the flow tube was exposed to ultra-violet light, especially when the irradiation was done near the downstream end (Nos. 31). This indicates that the rate of DMN photolysis must be more rapid than the rates of its formation in any photochemical processes which might occur in the flow tube under the prevailing conditions. In order to distinguish between DMN formed *in situ* by conversion of DMA adsorbed on the Tenax cartridge and DMN formed from DMA flowing through the tube, a series of experiments were carried out in which air containing $^{2}H_{6}$-DMA, NO_x, and ozone was passed through the flow tube and sampled with a cartridge which had been preloaded with $^{1}H_{6}$-DMA (Nos. 32-34). Approximately three times as much $^{2}H_{6}$-DMN as $^{1}H_{6}$-DMN was found. This experiment was repeated in reverse fashion, with $^{1}H_{6}$-DMA being collected on a cartridge preloaded with $^{2}H_{6}$-DMA (Nos. 35 and 36), and the amount of $^{1}H_{6}$-DMN collected was more than double the $^{2}H_{6}$-DMA formed on the cartridge. In these experiments the amount of DMA passing through the flow tube was not as precisely known as the amount which was preloaded on the cartridges. The reason for this is that the temperature at the upstream end of the flow tube was not thermostatically controlled. Likewise, the room temperature permeation rates were not determined under thermostatic control. However, the resulting uncertainty in the concentration of DMA in the air flowing through the tube could not account for the extent to which the quantity of DMN formed in the flow tube exceeded the quantity formed on the cartridge. It is apparent that formation of DMN from NO_2, ozone, and DMA is *less efficient* in a Tenax cartridge bed than it is in a glass flow tube. Unfortunately, these experiments did not permit a clear distinction between homogeneous gas phase reactions such as might occur in the open air and heterogeneous reactions occurring on the wall of the flow tube.

To determine the extent to which DMN that had formed in the reaction tube might have adhered to the glass wall, samples were taken after the flow tube experiments had been completed and the permeation tube had been removed. In preparation, the reaction tube was cleaned by heating it from ambient to 75°C over a period of 30 minutes while passing 5 ℓ/min of air through it. During this time a 30 ℓ sample was taken on a Tenax cartridge at the downstream end of the tube. ${}^{2}H_6$-Dimethylamine had last been passed through the tube eight days before. During the intervening time the tube had been used for several other experiments. When the cartridge was desorbed and analyzed for ${}^{2}H_6$-DMN, 7.84 nM were found. A second 30 ℓ sample was then taken (30 min sampling period) while the tube was maintained at 75°C to confirm that it had been purged free of ${}^{2}H_6$-DMN and none was found. The tube was cooled to room temperature and ${}^{2}H_6$-DMA, NO_2 and ozone was passed through it for one hour. Following this a 5 ℓ/min stream of clean air was again passed for 48 min while the temperature was raised to 75°C and a 45 ℓ sample was collected on a Tenax cartridge. On this cartridge only 0.20 nM of ${}^{2}H_6$-DMN were found. The amount of DMN that was retained during any of the experiments in Table 22 was probably small, since only a small quantity of DMN was recovered by stripping immediately after passing DMA through the tube for an hour. Since a much larger quantity of DMN was accumulated on the tube during four days of passing D_6-DMN through it, and since a substantial amount remained on the tube for eight days afterward, it would appear that desorption of DMN from a glass surface is a very slow process at room temperature. This means that (1) only a small amount of DMN is lost during the course of an experiment by adsorption on the tube, and (2) desorption of DMN from the tube at ambient temperature is too low to significantly affect the results of subsequent experiments. This further implies that either most of the DMN is formed in homogeneous, gas-phase reactions or that heterogeneous formation of a molecule of DMN does not usually result in its adsorption.

The results obtained in this study show that it is important to obtain simultaneous data on atmospheric concentrations of NO_x, O_3, and amines when sampling for nitrosamines. This would be especially necessary to any attempt to show that nitrosamines had been formed in the atmosphere from reactants.

SUMMARY

Although establishing the presence and quantity of DMN in ambient air has been the first emphasis of this study, it is also important to realize that this compound is one of many present in the pollution profile. Characterization of the other components of the air mixture is of vital importance. The complete characterization of this mixture is essential for valid epidemiological correlations between compound incidence and incidence of neoplasm. Also essential for epidemiological correlations, in addition to identification of compounds present, is an indication of their quantities present and work on this important aspect of the problem is the subject of future research.

SECTION 10

DETECTION OF N-NITROSOAMINES UTILIZING SELECTED M/E IONS VIA COMPUTER SEARCH OF GC/MS/COMP DATA OBTAINED ON AMBIENT AIR SAMPLES

A computer search was conducted for N-nitrosoamine compounds in ambient air samples which were collected over a period of 15 months from various geographical areas within the continental U.S. Mass spectral data of organic vapors in ambient air had been accumulated on magnetic tapes and these data were examined for nitrosoamine compounds. Mass spectra were surveyed for the following N-nitrosoamine compounds: N-nitrosodimethylamine, N-nitrosodiethylamine, N-nitrosodi-n-butylamine, N-nitrosopiperidine, N-nitrosopyrrolidine, N-nitrosomorpholine, N-nitrosohexamethylimine, N-nitrosomethylcyclohexylamine, N-nitrosomethylbenzylamine, and N-nitrosomethylphenylamine.

EXPERIMENTAL

Sampling Techniques

During a 15 month period, cartridges were used for concentrating organic vapors on a 1.5 x 6.0 cm bed of Tenax GC (35/60) in a glass sampling cartridge.(1) All sampling cartridges were preconditioned by heating to 275°C for a period of 20 minutes under a helium purge of 20-30 ml/min. After cooling in precleaned Kimax® culture tubes, containers were sealed to prevent contamination of the cartridge during transportation and storage. Sampling cartridges prepared in this manner were carried by automobile or air freight to the sampling site. Two to three cartridges were designated as blanks to determine whether any of the cartridges might have been contaminated by the packing and transportation procedure. Cartridges containing known quantities (100/300 ng) of N-nitrosodimethylamine were in some cases prepared and carried to and from the field, stored and analyzed to determine recovery of N-nitrosodimethylamine.

Samples were taken in replicate as well as blanks discussed above were subjected to analysis by capillary gas chromatography/mass spectrometry/computer (Figure 6). Thermal desorption was used to transfer the entire amount of trapped vapors from the cartridge sampler to the analytical systems and required a specially designed manifold.(1-4) In a typical thermal desorption cycle, a sampling cartridge was placed in the preheated (~270°C) desorption chamber and helium gas was channeled through the cartridge (~20 ml/min) to purge the vapors into the liquid nitrogen cooled capillary trap. After desorption, the six-port valve was rotated and the temperature on the capillary loop was rapidly raised (>10° per min). The carrier gas introduced the vapors onto the glc column.

A Varian MAT CH-7 glc/ms/comp system was used to perform analysis (Figure 13). The operating parameters used on the glc/ms/comp system for analysis of samples collected at various geographical areas was given in Table 23. Ambient air samples collected as described above were analyzed on a 400 ft stainless steel SCOT or a 100 m glass SCOT both were coated with OV-101. Desorption of ambient air pollutants (including nitrosoamines) from the Tenax cartridges was achieved at 270°C. A single stage glass jet separator interfaced the SCOT capillary columns to the mass spectrometer and was maintained at 220°C.

Typically the mass spectrometer was first set to operate in the repetitive scanning mode. In this mode, the magnet was automatically scanned upward from a preset low mass to high mass value. Although the scan range may vary depending on the particular sample typically the range was from m/e 28 to m/e 400. The scan was completed in ~3 sec. The instrument then reset itself to the low mass position in preparation for the next scan and the information was accumulated by on-line 620/L computer onto magnetic tapes. The reset period required ~3 sec. Thus, a continuous scan cycle of ~6 sec/scan was maintained.

Prior to running known samples, the system was calibrated by introducing a standard substance, such as perfluorokerosene into the instrument and determining the time of appearance of the known standard peaks in relation to the scanning magnetic field. The calibration curve which was generated was stored in the 620/L computer memory.

With the magnet continuously scanning the sample was injected and automatic data acquisition was initiated. As each spectrum was acquired by the computer, each peak which exceeds the preset threshold was recognized and reduced to centroid time and peak intensity. This information was stored in the computer core while the scan was in progress. In addition,

Table 23. OPERATING PARAMETERS FOR GLC-MS-COMP SYSTEM

Parameter	Setting
Inlet-manifold	
desorption chamber	270°C
valve	220°C
capillary trap - minimum	-195°C
maximum	+180°C
thermal desorption time	4 min
GLC 100 m glass SCOT OV-101	20-240°C, 4/C° min
400 ft SS SCOT OV-101	20-240°C, 4/C° min
carrier (He) flow	~3 ml/min
transfer line to ms	240°C
MS	
scan range	m/e 20 → 300
scan rate, automatic-cyclic	1 sec/decade
filament current	300 μA
multiplier	6.0
ion source vacuum	$\sim 4 \times 10^{-6}$ torr

~30 TIC values and an equal number of Hall probe signals were stored in core as they were acquired. During the 3 sec period between scans, this spectral information, along with the spectrum number was written sequentially on the magnetic tape and the computer was reset for the acquisition of the next spectrum.

This procedure continued until the entire gc run was completed. By this time, there were from 300-1000 spectra per chromatographic run which were then subsequently processed. Depending on circumstances, the data was either processed immediately or additional samples were run, stored on magnetic tape and the results examined at a later time.

The mass spectral data was processed in the following manner. The original spectra was scanned and the TIC information was extracted. Then the TIC intensities were plotted against the spectrum number on the STATOS I Recorder. The information was generally indicative of whether the run was suitable for further processing since it gave some idea of the number of unknowns in the sample and the resolution obtained using the particular glc column conditions.

The next stage of the processing was the mass conversion of the spectral peak times to peak masses which was done directly by a computer disk system. Mass conversion was accomplished by use of the calibration table obtained previously. Normally one set of calibration data was sufficient for an entire days data processing since the characteristics of the Hall probe are such that variation and calibration was less than 0.2 atm/day. A typical time required for this conversion process for 1,000 spectra was approximately 45 minutes.

After the spectra were obtained in mass converted form, processing proceeded either manually or by computer.

The technique of mass fragmentography was used for the resolution and detection of N-nitrosoamines in ambient air samples. This method consists of acquiring full mass spectra as described above during the chromatographic separation step and then using selected ions which are presented as mass fragmentograms with the aid of computer software programs. This allowed the possibility of resolving and detecting constituents not visually apparent from the total ion current chromatogram. In our gc/ms/comp system it is possible to request from the Varian 620/L dedicated computer mass fragmentograms for any combination of m/e when full mass spectra are obtained during chromatography. Thus, selectivity can be achieved by selecting the unique ion for that particular compound specifically nitrosamines which are presented as intensity *vs*. time and using ion intensity for quantitation. Table 24 depicts the nitrosamines and their m/e ions selected for detection in ambient air samples. Listed in this table are the parent ions for each of the compounds and then the ions of first, second, third and fourth choice in decreasing order of importance which were utilized for the purpose of detection and/or quantitation of the N-nitrosoamines. For example, N-nitrosodimethylamine the parent ion (m/e 74) was selected as the first choice ion for representation in mass fragmentography since it represents a rather unique ion of high intensity. In this manner, mass fragmentograms for each of the ions listed in Table 24 were generated by the computer system and plotted in terms of ion intensity *vs* chromatographic time. By

Table 24. NITROSAMINES AND THEIR M/E IONS SELECTED FOR DETECTION IN AMBIENT AIR SAMPLES

Compound	Parent m/e	m/e (I)[a]			
		1st	2nd	3rd	4th
N-nitrosodimethylamine	74	74 (100)	42 (67)	-	-
N-nitrosodiethylamine	102	102 (57)	56 (53)	42 (98)	44 (100)
N-nitrosodi-n-butylamine	158	84 (80)	158 (17)	115 (16)	70 (14)
N-nitrosopiperidine	114	114 (48)	42 (100)	69 (5)	-
N-nitrosopyrrolidine	100	100 (50)	69 (27)	-	-
N-nitrosomorpholine	116	116 (38)	56 (100)	86 (28)	-
N-nitrosohexamethyleneimine	128	128 (58)	69 (32)	-	-
N-nitrosomethylcyclohexylamine	142	142 (79)	67 (22)	125 (13)	-
N-nitrosomethylbenzylamine	150	150 (9.5)	63 (8)	-	-
N-nitrosomethylphenylamine	136	79 (22)	104 (14)	136 (11)	-

[a] I = intensity of fragment ion in the mass spectrum.

observing the retention time for standard, authentic nitrosamines chromatographed under similar operating conditions, a search for the nitrosamines in the ambient air samples was made.

The overall sensitivity of the mass fragmentographic technique for nitrosamines in ambient air is shown in Table 25. The sensitivity levels depicted here are only approximations which are based on (a) the detection of the primary (first choice) selected m/e ion by the mass spectrometer, (b) the breakthrough volume of each nitrosamine at the ambient air temperature during sampling, and (c) other instrumental operating parameters.

RESULTS AND DISCUSSION

Tables 26-32 lists the ambient air samples from the various geographical areas within the continental U.S. that were examined for nitrosamines by mass fragmentography. These included the Houston, TX vicinity, Los Angeles, CA basin, the Kanawha Valley, WV, St. Louis, MO, Denver, CO, Atlanta and Macon, GA and Baltimore, MD. Although these samples had been primarily collected at these various sites for the purpose of identifying other organic vapor pollutants, mass fragmentography could and was applied to the detection of nitrosamines.

A survey of all of these samples indicated the presence of N-nitrosodiethylamine in a sample taken from the Eisenhower Tunnel in Colorado (Table 31). A trace of N-nitrosodimethylamine was also tentatively detected. Figure 29 depicts the mass fragmentogram for N-nitrosodiethylamine obtained for this sample. It was estimated that the concentration of N-nitrosodiethylamine was ∿100 ppt. The examination of the remaining mass spectral data obtained on ambient air from the other remaining sites did not reveal the presence of N-nitrosoamines down to the levels of sensitivity for which the instrumentation was capable.

N-nitrosodimethylamine was detected and quantitated in ambient air from an industrial site in Baltimore, MD (Table 33) and the Kanawha Valley, WV (Table 34). These data have been reported in Section IX. A search in these samples for the presence of other nitrosamines was conducted and none were found.

Table 25. ESTIMATED OVERALL SENSITIVITY OF GC/MS/COMP TECHNIQUE FOR NITROSAMINES IN AMBIENT AIR

Compound	parts-per-trillion[a]
N-nitrosodimethylamine	150
N-nitrosodiethylamine	30
N-nitrosodi-n-butylamine	10
N-nitrosopiperidine	5
N-nitrosopyrrolidine	<5
N-nitrosomorpholine	<5
N-nitrosohexamethylene imine	<5
N-nitrosomethylcyclohexylamine	<5
N-nitrosomethylbenzylamine	<5
N-nitrosomethylphenylamine	<5

[a] Values are based upon the detection of the primary selection ion, its breakthrough volume (when known) at an ambient temperature of 70°F, and other instrumental operating parameters.

Table 26. AMBIENT AIR SAMPLING PROTOCOL FOR HOUSTON, TX AND VICINITY

Site	Sampling Location	Sampling Time (min)	Sampling Volume (ℓ)	Remarks	
Houston, TX (S1)	May St.	1,440	20,600	11/6-7/74 70°F	1630-1630 SE/2-5 mph
Houston, TX (S2)	Stuebner Airline	1,440	20,600	11/8-9/74 72°F	1030-1030 SE/5 mph
Pasadena, TX (S3)	Shaw Drive	1,440	20,800	11/11-12/74 64°F	1130-1130 NW/10-12 mph
Texas City, TX (S4)	-	1,440	21,000	11/12-13/74 64°F	1415-1415 NW/10 mph
Baytown, TX (S5)	7200 Bayway Drive	1,440	21,000	11/13-14/74 64°F	1630-1630 5/10-12 mph

Table 27. AMBIENT AIR SAMPLING PROTOCOL FOR LOS ANGELES, CA AND VICINITY

Site	Sampling Location	Sampling Time (min)	Sampling Volume (ℓ)	Remarks	
Santa Monica, CA (S1)	2441 Arizona Ave.	490	7,200	3/31/75 55°F	0850-1700 W/10 mph
West Covina, CA (S2)	820 Phillips St.	255	5,600	4/1/75 58°F	1000-1615 W/5 mph
Glendora, CA (S3)	840 E. Laurel	660	13,500	4/2/75 70°F	1000-2100 calm
Anaheim, CA (S4)	1700 E. Broadway	450	6,750	4/3/75 70°F	0930-1630 calm
Garden, Grove, CA (S5)	12281 Nelson St.	450	6,750	4/4/75 58°F	0900-1630 W/5 mph
Santa Monica, CA (S6)	2441 Arizona Ave.	900	16,200	3/31-4/1/75 55°F	1700-0800 calm

Table 28. SAMPLING PROTOCOL FOR THE KANAWHA VALLEY, WV

Site	Sampling Location	Sampling Time (min)	Sampling Volume (ℓ)	Remarks
S. Charleston (S1)	167 11th Ave.	480	2,097	8/4/75 0900-1700 85°F calm
S. Charleston (S2)	314 4th Ave.	480	2,036	8/4/75 1000-1750 85°F calm
Belle (S3)	1511 W. Central St.	480	2,040	8/5/75 1024-1830 85°F calm
Belle (S4)	Marmet Locks	480	2,026	8/5/75 0931-1751 82°F calm
Nitro (S5)	20th St. (Fire Station)	540	2,170	8/6/75 1031-1948 76°F WSW/2 mph
Nitro (S6)	4019 40th St.	540	2,240	8/6/75 1100-1900 78°F calm
St. Albans (S7)	6500 MacCorkle Ave. S.W.	720	2,310	8/7/75 1000-2000 77°F N/5 mph
St. Albans (S8)	7124 1/2 MacCorkle Ave. S.W.	480	2,222	8/7/75 1042-2035 77°F N/1-5 mph
S. Charleston (S9)	314 4th Ave.	510	2,086	8/8/75 0931-1800 70°F ENE/2-3 mph
S. Charleston (S10)	167 11th Ave.	450	1,652	8/8/75 0852-1628 70°F E/2-3 mph

Table 29. AMBIENT AIR SA[illegible]G PROTOCOL FOR HOUSTON, TX AND VICINITY

Site	Sampling Location	Sampling Time (min)	Volume Sampled (ℓ)	Remarks	
Pasadena, TX (S1)	C. H. Milby Park	260	1,534	8/29/75 100°F SE/10-15 mph	1005-1425 90% RH
Pasadena, TX (S2)	Mae St.	1,440	6,288	8/25-26/75 95°F SE/5 mph	1000-1000 87% RH
Pasadena, TX (S3)	Shaw Drive	1,440	3,976	8/26-27/75 81°F SE/5-7 mph	1000-1000 87% RH
Pasadena, TX (S4)	Shaw Drive	660	5,768	8/26/75 88°F SE/5-10 mph	1100-2230 99% RH
Pasadena, TX (S5)	Mae St.	450	1,890	8/25/75 95°F SE/5-10 mph	1430-2200 99% RH
Texas City, TX (S6)	Connie #10	1,440	2,338	8/27-28/75 80°F SE/5-10 mph	2235-1155 90% RH
Texas City, TX (S7)	Connie #10	635	2,058	8/27/75 80°F SE/5-10 mph	1200-2235 90% RH
Pasadena, TX (S8)	Shaw Drive	720	2,492	8/26-27/75 82°F SE/10 mph	2230-1017 93% RH

(continued)

Table 29 (cont'd)

Site	Sampling Location	Sampling Time (min)	Volume Sampled (ℓ)	Remarks	
Houston, TX (S9)	May St.	720	2,002	8/23/75 87°F SE/2-5 mph	1245-1200 92% RH

Table 30. AMBIENT AIR SAMPLING PROTOCOL FOR ST. LOUIS, MO AND VICINITY

Site	Sampling Location	Sampling Time (min)	Sampling Volume (ℓ)	Remarks
Alton, Il (S1)	2421 Chris Lisa St.	540	1,898	9/11/75 2250-0750 69°F NW/7-10 mph
Wood River, Il (S2)	2 mi East of Shell Refinery	300	966	9/11/75 1256-1756 79°F W/10-20 mph
Arvado, MO (S3)	4400 Lindell	360	1,130	9/10/75 0650-1250 81°F calm
Arvado, MO (S4)	4400 Lindell	527	1,582	9/9/75 2212-0635 82°F calm
St. Ann (S5)	St. Charles Rd. and Industrial Blvd.	415	2,028	9/8/75 2035-0525 88°F WS/2 mph
Webster Grove, MO (S6)	Mary St.	360	1,000	9/9/75 1114-1604 93°F W/0-5 mph

Table 31. AMBIENT AIR SAMPLING PROTOCOL FOR DENVER, CO AND VICINITY

Site	Sampling Location	Sampling Time (min)	Sampling Volume (ℓ)	Remarks	
I-70, Colorado (S1)	Eisenhower Tunnel	566	3,360	9/18/75 40°F	2024-0550 WNW/5 mph
I-70, Colorado (S2)	Eisenhower Tunnel	405	2,116	9/18/75 65°F	1239-1924 SW/20 mph
Rocky Mtn. Park, CO (S3)	Trail Ridge Rd.	484	2,590	9/17/75 49°F	0955-1759 WSW/30 mph
Arvado, CO (S4)	W. 57 Ave & Garrison	481	2,968	9/16/75 72°F	2159-0700 SW/7 mph
Arvado, CO (S5)	W. 47 Ave & Garrison	470	2,780	9/16/75 ~80°F	1348-2138 WNW/1-7 mph
Welby, CO (S6)	78th Ave. & Steele St.	300	2,284	9/15/75 ~63°F	1230-0650 calm
Denver, CO (S7)	16th Ave & Park	360	2,105	9/15/75 91°F	1200-1800 WS/2 mph

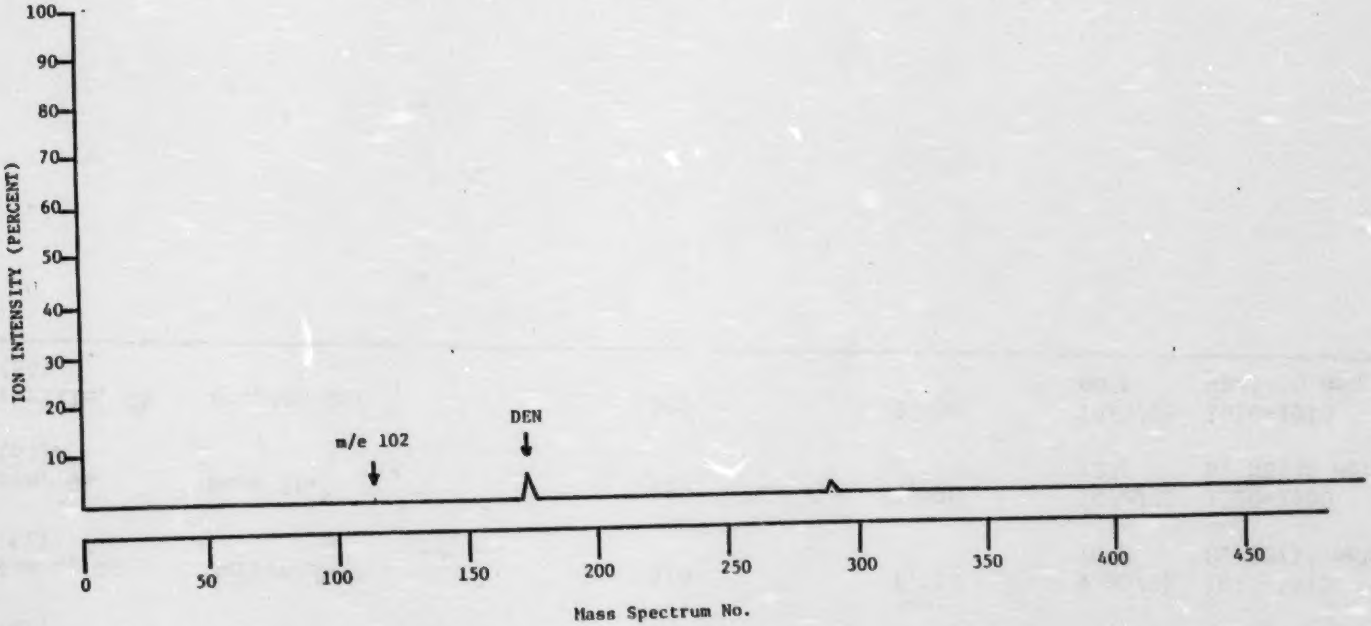


Figure 29. Mass fragmentogram at m/e 102 for N-nitrosodiethylamine.

Table 32. AMBIENT AIR SAMPLING PROTOCOL FOR ATLANTA AND MACON, GA

Site	Sampling Location	Sampling Time (min)	Sampling Volume (ℓ)	Remarks
Atlanta, GA (S1)	248 Oakland Ave. S.E.	270	2,120	9/29/75 1130-1600 70°F NE/15 mph
Atlanta, GA (S2)	Jefferson St.	310	1,710	9/30/75 1045-1555 70°F E, SE/15 mph
Macon, GA (S3)	Mead St.	280	1,270	10/2/75 1120-1600 72°F N, NE/15 mph
Doraville, GA (S4)	Dresden Dr.	305	2,290	10/3/75 1010-1515 60°F NE/5-10 mph

Table 33. SAMPLING PROTOCOL FOR BALTIMORE, MD AND VICINITY

Site	Sampling Location	Sampling Time (min)	Sampling Volume (ℓ)	Remarks	
Baltimore, MD	North Bridge and Fairfield (Parking Lot)	210	300	10/14/75 85°F	1100-1450 W/8 kts
Baltimore, MD	North Bridge and Fairfield (Parking Lot)	210	300	10/14/75 81°F	1500-1850 WNW→WSW/5 kts
Baltimore, MD	North Bridge and Fairfield (Parking Lot)	210	300	10/14/75 73°F	1900-2250 SW/Variable
Baltimore, MD	North Bridge and Fairfield (Parking Lot)	210	300	10/14-15/75 62°F	2300-0250 Variable
Baltimore, MD	Patapsco Sewage Treatment Plant (End of North Bridge)	210	300	10/16/75 70°F	1000-1350 NW/9 kts
Baltimore, MD	Patapsco Sewage Treatment Plant (End of North Bridge)	210	300	10/16/75 72°F	1400-1750 NW/9 kts
Baltimore, MD	Chessie Coal Piers	210	300	10/17/75 56°F	1410-1800 ENE/7-14 kts
Baltimore, MD	North Bridge and Fairfield) (WNW of Diamazine Plant)	120	120	10/19/75 65°F	1400-1600 E/3 kts

(continued)

Table 33 (cont'd)

Site	Sampling Location	Sampling Time (min)	Sampling Volume (ℓ)	Remarks	
Fairfield, MD	Conoco Parking Lot	120	120	11/20/75 66°F	1545-1745 SWS/3-6 kts
Baltimore, MD	North of FMC (Near Memirac Corp.)	120	120	11/20/75 57°F	2020-2220 SSW/4 kts

Table 34. AMBIENT AIR SAMPLING PROTOCOL FOR KANAWHA VALLEY, WV

Site	Location	Sampling Time (min)	Volume Sampled (L)	Remarks
Belle, WV	DuPont Plant (1)	285	247	12/1/75 2132–0217 30–35°F NW/1 kt
Belle, WV	DuPont Plant (2)	292	275	12/1/75 2127–0219 30–35°F NW/2 kts
Belle, WV	DuPont Plant (3)	293	255	12/1/75 2216–0309 30–35°F NW/2 kts
Belle, WV	DuPont Plant (4)	300	294	12/1/75 2207–0307 30–35°F NW/2 kts
Belle, WV	DuPont Plant (1)	261	243	12/2/75 0229–0652 30°F SE/4 kts
Belle, WV	DuPont Plant (2)	263	341	12/2/75 0228–0653 30°F SE/4 kts
Belle, WV	DuPont Plant (3)	191	297	12/2/75 0400–0711 30°F SE/4 kts
Belle, WV	DuPont Plant (4)	235	336	12/2/75 0317–0712 30°F SE/4 kts
Belle, WV	DuPont Plant (2)	362	320	12/2/75 0900–0302 40–50°F SE/2–calm
Belle, WV	DuPont Plant (3)	320	350	12/2/75 2202–0318 40°F SE/2 kts
Belle, WV	DuPont Plant (4)	295	406	12/2/75 2205–0300 40°F SE/2 kts

(continued)

Table 34 (cont'd)

Site	Location	Sampling Time (min)	Volume Sampled (ℓ)	Remarks
S. Charleston, WV	Union Carbide (9)	232	248	12/3/75 1441-1801 50-55°F WNW-NW/2 kts
S. Charleston, WV	Union Carbide (10)	120	350	12/3/75 1512-1712 50-55°F WNW→NW/2 kts
S. Charleston, WV	Union Carbide (11)	171	294	12/3/75 1536-1827 50-55°F WNW→NW/2 kts
S. Charleston, WV	Union Carbide (12)	120	292	12/3/75 1538-1728 50-55°F WNW→NW/2 kts
S. Charleston, WV	Union Carbide (11)	200	502	12/3/75 1833-2053 45-50°F NW-N/2 kts
S. Charleston, WV	Union Carbide (9)	182	401	12/3/75 1816-2019 45-50°F NW→N/2 kts
S. Charleston, WV	Union Carbide (13)	122	392	12/3/75 1751-1956 45-50°F NW→N/2 kts
S. Charleston, WV	Union Carbide (14)	140	521	12/3/75 1815-2040 45-50°F NW→N/3 kts
S. Charleston, WV	Union Carbide (11)	150	502	12/3/75 1833-2053 45-50°F NW→N/3 kts

(continued)

Table 34 (cont'd)

Site	Location	Sampling Time (min)	Volume Sampled (ℓ)	Remarks
S. Charleston, WV	Union Carbide (13)	135	402	12/3/75 2003-2217 40-45°F N→NNE/3 kts
S. Charleston, WV	Union Carbide (14)	117	325	12/3/75 2047-2244 40-45°F N→NNE/3 kts
Belle, WV	DuPont Plant (5)	119	243	12/4/75 1710-1911 54-60°F NE/2 kts
Belle, WV	DuPont Plant (6)	118	256	12/4/75 1526-1724 60°F NE/2 kts
Belle, WV	DuPont Plant (7)	125	281	12/4/75 1600-1805 60°F calm
Belle, WV	DuPont Plant (8)	120	348	12/4/75 1906-2106 60°F NE/2 kts
Nitro, WV	I-60 and WV25	230	1,593	12/5/75 1158-1548 65°F SW/10 kts
Nitro, WV	I-60 and WV25	240	1,800	12/5/75 1159-1549 65°F SW/10 kts

SECTION 11

IDENTIFICATION OF VOLATILE ORGANIC VAPORS IN AMBIENT AIR FROM SEVERAL GEOGRAPHICAL AREAS IN THE CONTINENTAL U.S.

The overall objective was to apply the sampling and analytical methodology to the analysis of ambient air pollutants. Our specific objectives has been to determine the viability of this technique for the collection and analysis of various chemical classes occurring in the atmosphere. In order to demonstrate the utility of this methodology, various geographical areas within the Continental U.S. were selected for study. The selection of these areas was based on two primary factors. The first was related to the types of industrial activity which were cited in the Chemical Industry Directory on a state by state basis which indicated the potential types of organic vapors that might be present in the atmosphere due to the type of chemical activity occurring at these sites. Selection of sites was based on the activity in which the industry was engaged, e.g. whether it was involved in the production, the use, or storage of volatile organic chemicals. These activities were related to the storage, use or production of chlorinated hydrocarbons, nitrogenous substances, oxygenated materials, and sulfur compounds. A second criteria used in the selection of study areas was the relationship between the heavy industrial activity and the high incidence of cancer which has been demonstrated by statistical studies reported by the National Cancer Institute.(14)

The geographical areas which were studied under this program were: the Kanawha Valley in West Virginia, Houston, TX and vicinity, St. Louis, MO, Denver, CO, Atlanta, GA and vicinity, Central and Northern New Jersey, and the Los Angeles, CA Basin.

EXPERIMENTAL

Sampling Techniques

The sampling procedure employed has been previously described(1) which consisted of concentrating hazardous vapors and other organic compounds on a 1.5 x 6 cm bed of Tenax GC (35/60) in a glass cartridge. All sampling cartridges were preconditioned by heating to 275°C for a period of 20 min under a Helium purge of 20-30 ml/min. After cooling in precleaned Kimax® culture tubes, the containers were sealed to prevent contamination of the cartridge. Sampling cartridges were carried by air freight or automobile to the sampling site with 2-3 cartridges designated as blanks to determine whether any of the cartridges might be contaminated by the packing and transportation procedure. Ambient air samples were collected with a Nutech Model 221-A AC/DC portable sampler.(1) In general, a sampling rate of 1-2 ℓ/min/cartridge was used throughout this study.

Meterological conditions were recorded with hand held instruments. The wind direction, velocity, temperature and humidity were all determined. Wind direction was determined using a lensatic compass. The compass was also used to describe the sampling location relative to major industrial facilities. Wind velocity was estimated with a Dwyer wind meter (Dwyer Instruments Inc., Michigan City, IN), a hand held rotameter with two scales, 2-10 mph and 4-66 mph. Barometric pressure was measured with a Pocket Altimeter (Gischard, West Germany). This aneroid barometer was compared with a mercury barometer and found to read to 0.1 in of mercury too high. It was calibrated from 19-31" of mercury and 0-13,000 ft of altitude. Air temperature and relative humidity were determined with a sling psychrometer (Taylor Instruments Co., Rochester, NY). Precipitation was measured volumetrically with a Nimbus Model 609-B rain gauge (Air Guide Instruments Co., Chicago, IL).

Distances from a suspected point source of pollution or for determining the location of sampling was estimated with a Rangematic Distance Finder (Ranging Inc., Rochester, NY). The range finder was calibrated for 50-1,000 yds (also has indications for 1 and 2 miles). It was found to be accurate to ±1% at 100 yds.

The sampling protocols employed for ambient air analysis in the various geographical areas within the Continental U.S. were given in Tables 26-35. Sampling locations for the Los Angeles, CA basin are depicted in Figures 30 and 31.

Instrumental Methods of Analysis

The instrumental system (glc/ms/comp) used for the qualitative and quantitative analysis of organic vapors and the inlet-manifold used for recoverying vapors trapped on Tenax GC sampling cartridges has been

Table 35. SAMPLING PROTOCOL FOR CENTRAL AND NORTHERN NEW JERSEY AND LOS ANGELES, CA BASIN

Site	Sampling Location	Sampling Time (min)	Sampling Volume (ℓ)	Remarks
Paterson, NJ (S1)	12th St. & 4th Ave.	42	300	3/22/76 1231-1313 hr 40°F 300-360°/3 mph
Clifton, NJ (S2)	Dyer Ave. & Wheeler St.	39	300	3/22/76 1528-1607 hr 45°F 320°/2 mph
Passaic, NJ (S3)	First St. & Essex St.	39	300	3/22/76 1715-1754 hr 40°F 320°/5 mph
Hoboken, NJ (S4)	New County Rd. U. S. Post Office Depot	39	300	3/23/76 1223-1302 hr 51°F 230°/0-10 mph
Newark, NJ (S5)	552 Doremus Ave.	38	300	3/23/76 1400-1438 hr 53°F 270°/0-10 mph
New York City, NY (Staten Island) (S6)	Chelsea Rd. at Bloomfield Ave.	37	300	3/23/76 1702-1739 hr 54°F 280°/0-5 mph
Edison, NJ (S7)	Meadow Rd., directly across from Stauffer plant	42	300	3/25/76 1720-1802 hr 62°F 225-240°/3-8 mph
Fords, NJ (S8)	North of Tenneco plant	44	300	3/26/76 1559-1643 hr 72°F 200°/0-2 mph

(continued)

Table 35 (cont'd)

Site	Sampling Location	Sampling Time (min)	Sampling Volume (ℓ)	Remarks
Bound Brook, NJ (S9)	Eastern Turnpike directly north of American Cyanamid Co.	44	300	3/26/76 1732-1816 hr 68°F 200°/0-7 mph
El Segundo, CA (S1)	Illinois St. (See Fig. 30)	54	300	5/12/76 1329-1423 hr 76°F 220-240°/2-8 mph
Torrance, CA (S2)	19146 Van Ness Blvd.	55	300	5/13/76 1307-1412 hr 76°F 230-250°/2-7 mph
Los Angeles, CA (S3)	20100 Normandie Ave.	54	300	5/13/76 1357-1451 hr 78°F 270°/0-7 mph
Long Beach, CA (S4)	63rd Avenue & Paramount Blvd.	52	300	5/13/76 1707-1759 hr 80°F 250°/3-8 mph

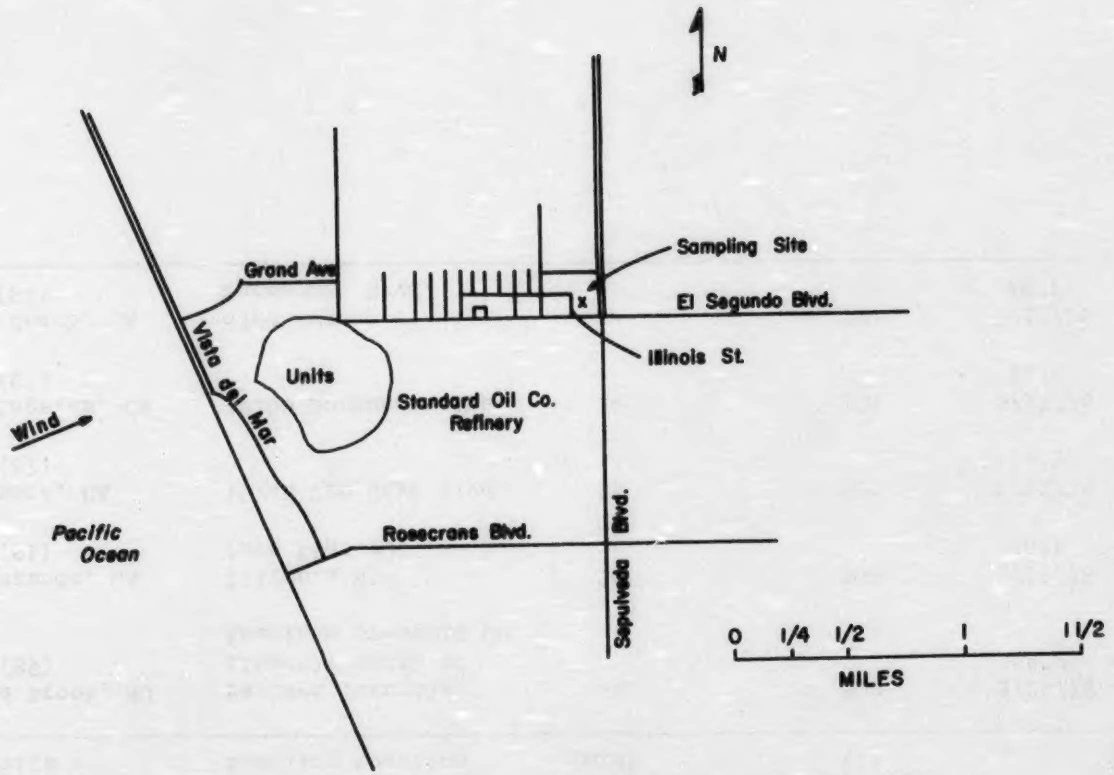

N
Sampling Site
Grand Ave
El Segundo Blvd.
x
Illinois St.
Vista del Mar
Units
Standard Oil Co. Refinery
Wind
Pacific Ocean
Rosecrans Blvd.
Sepulveda Blvd.
0
1/4
1/2
1
1 1/2
MILES

Figure 30. Map depicting sampling site in El Segundo, CA

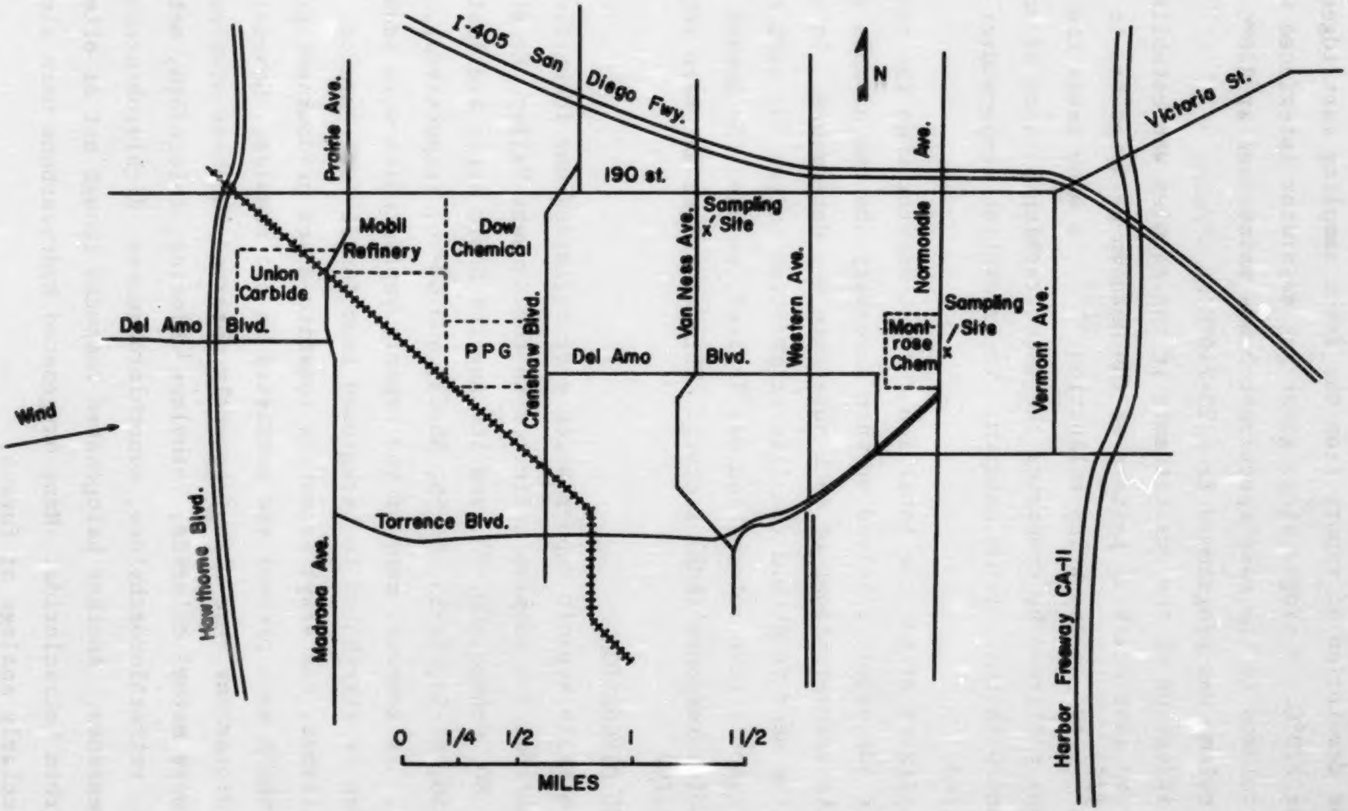

I-405 San Diego Fwy.
Victoria St.
N
190 st.
Prairie Ave.
Mobil Refinery
Dow Chemical
Union Carbide
Del Amo Blvd.
PPG
Crenshaw Blvd.
Del Amo Blvd.
Van Ness Ave.
Sampling x Site
Western Ave.
Normandie Ave.
Sampling x Site
Mont-rose Chem
Vermont Ave.
Harbor Freeway CA-11
Hawthorne Blvd.
Madrona Ave.
Torrance Blvd.
Wind
0
1/4
1/2
1
1 1/2
MILES

Figure 31. Map depicting sampling site in Torrance, CA

previously described.(1,18) The operating parameters for the glc/ms/comp system for the analysis of samples was given in Table 23. Samples were analyzed on a 100 m glass SCOT capillary coated with OV-101 stationary phase. The desorption of vapors from the Tenax sampling cartridges was achieved at 270°C. A single stage glass jet separator interfaced with SCOT capillary columns to the mass spectrometer was maintained at 220°C. The capillary column was programmed from 20-240°C at 4°/min.

Identification of the constituents in the samples was established by comparing the mass cracking pattern of the unknown mass spectra to an 8 peak index(12) and to the Wiley collection.(13) In many cases the identification was confirmed by comparing the mass cracking pattern of an authentic compound with that of the unknown. Their elution temperatures were also compared.

By utilizing either the total ion current monitor when the constituents were adequately resolved or when necessary the use of mass fragmentograms, the concentrations of each substance was determined. In order to eliminate the need to obtain complete calibration curves for each compound for which quantitative information was desired, we used the method of relative molar response (RMR) factors. This technique has been reported elsewhere.(20)

RESULTS AND DISCUSSION

The volatile organic vapors which were collected and identified utilizing glc/ms/comp for samples collected in the Kanawha Valley, Houston, TX, St. Louis, MO, Denver, CO, NJ, and Los Angeles Basin areas are listed in Tables 38-40, 41-50, 51-53, 54-55, 56-63, and 64-66, respectively, in Appendix I. In general, many of the organic vapors which were identified probably can be attributed to background from fossil fuel burning. The alkanes, alkenes, and alkyl aromatics constitued the predominant group of compounds which were present and persisted in all samples. Several halogenated hydrocarbons were also frequently observed in these samples. These compounds were methyl chloride, methylene chloride, chloroform, methyl chloroform, tetrachloroethylene, monochlorobenzene, dichlorobenzenes and trichlorobenzenes. Another halogenated compound though not as often observed was carbon tetracloride. Many oxygenated hydrocarbons were also detected, particularly analogs of furans.

In ambient air samples from the C. H. Milby Park in Pasadena, TX, we identified 2-chloro-1,3-butadiene (chloroprene) and 1-chlorobutene-3-yne. These samples were taken a location approximately 200 yds downwind from an industrial complex. Ambient air samples collected at an upwind site during the same sampling period, did not reveal the presence of these two chlorinated hydrocarbons. A third unique chlorinated hydrocarbon, 1,4-dichloro-2-butene was tentatively identified in the sample collected at C. H. Milby Park. Ambient air samples collected in Pasadena, TX at locations S2 and S3 (see Table 29) were found to contain dibromodichloromethane and bromoform.

The presence of dimethylnitrosoamine was tentatively identified in ambient air samples collected at the entrance of the Eisenhower Tunnel in Colorado. N-nitrosodiethylamine was also detected in these samples which was previously described in Section X. An additional nitrogenous compound dimethylformamide was also identified.

Samples from the Central and Northern NJ area contained many compounds of particular interest. We identified several halogenated compounds. These were: dibromomethane, vinyl chloride, 1,2-dichloroethane, 1,1-dichloropropane, 2-chloroethyl acetate, N-decyl chloride and a chloropropane. Also many nitrogen containing compounds were detected. These were: ethylamine, isoamyl nitrile, pyridine, aniline, N-methylaniline, dimethylaniline, chloroaniline, α-naphthylamine and 2-ethylquinoline. The concentrations of several ambient air pollutants near industrial sites in the New Jersey area were quantitated. Their levels are given in Table 36. The concentration of vinyl chloride was approximately 120,000 ng/m^3 of ambient air. The concentration of chloroaniline in a sample taken from Bound Brook was 33 ng/m^3. In the same sample, a very high concentration of chlorobenzene was detected (20,000 ng/m^3). Whereas in many other samples that have been analyzed at several different geographical locations, generally indicate a trace to non-detectable levels of chlorobenzene (<10 ng/m^3). Table 36 presents a general trend which exemplifies the ubiquitous nature of many of the halogenated hydrocarbons *e.g.* chloroform has been consistently found at levels in the samples from New Jersey area to be in the μg/m^3 range. On the otherhand, the chlorobenzenes are in trace amounts. The highest concentration of all of the pollutants measured was methyl acrylate in Newark, NJ (4,545,000 ng/m^3). The same sample had a high

Table 36. CONCENTRATIONS OF AMBIENT AIR POLLUTANTS NEAR INDUSTRIAL SITES IN THE NEW JERSEY AREA[a]

Compound	Bound Brook	Paterson	Clifton	Fords	Newark	Passaic	Hoboken	Staten Is. (NY)
benzene	9,000	2,160	trace	3,068	300,000	2,045	trace	2,270
n-butyl acetate	ND	ND	ND	ND	113,000	ND	ND	ND
chloroaniline	33	ND	ND	ND	ND	ND	ND	ND
chlorobenzene	20,000	trace	trace	trace	trace	ND	trace	trace
chloroform	4,167	3,750	8,300	16,700	37,000	4,167	2,083	20,830
dibromoethane	ND	130	ND	ND	ND	ND	ND	ND
1,2-dichloroethane	trace	trace	64,516	ND	ND	ND	trace	ND
α-methylnaphthalene	134	ND	ND	ND	ND	ND	ND	ND
nitrobenzene	126	ND	ND	ND	ND	ND	ND	ND
tetrachloroethylene	trace	trace	trace	trace	trace	trace	trace	trace
1,2,4-trichlorobenzene	99	ND	ND	ND	ND	ND	ND	ND
1,3,5-trichlorobenzene	867	ND	ND	ND	ND	ND	ND	ND
1,1,1-trichloroethane	trace	trace	trace	1,300	trace	13,000	trace	trace
trichloroethylene	trace	1,200	trace	ND	ND	trace	trace	ND
vinyl chloride	ND	ND	400	ND	ND	$\sim$120,000	ND	ND
methyl acrylate	trace	ND	ND	ND	4,545,000	ND	ND	ND
n-butyl acrylate	ND	ND	ND	ND	17,000	ND	ND	ND

[a] Values in ng/m^3

concentration of benzene (300,000 ng/m^3), n-butyl acetate (113,000 ng/m^3), chloroform (37,000 ng/m^3) and n-butyl acrylate (17,000 ng/m^3). Benzene has been regarded as a ubiquitous pollutant since it has been detected at measurable quantities in the majority of samples which we have collected throughout the Continental U.S.

The concentrations of some pollutants which were identified in ambient air from Torrance, CA are given in Table 37 (Fig. 31). A rather high concentration of carbon tetrachloride was detected (38,095 ng/m^3) and methylene chloride (14,285 ng/m^3). This sample also contained m-chlorobenzaldehyde and chloral.

In Tables 38-66, many siloxane compounds have been indicated. These compounds are generally derived as background constituents from the high resolution capillary column used for effecting the separation of the mixtures. Also in some samples, the presence of ethylene oxide has been noted. This compound is believed to be derived as background from the sampling cartridge during the thermal desorption step.

Table 37. CONCENTRATION OF POLLUTANTS IN AMBIENT AIR IN TORRANCE, CA

Compound	ng/m^3
benzene	13,640
carbon tetrachloride	38,095
chlorobenzene	20,670
m-chlorobenzaldehyde	334
chloral	660
methylene chloride	14,285
1,2,3,3-tetrachloropropene	100
trichlorobenzene	2,670
1,1,1-trichloroethane	1,000
trichloroethylene	~1,000

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Luginbyhl, T. T.: editors. Carroll, B. S.: project coordinator. Suspected Carcinogens. Subfile of NIOSH Toxic Substances List. U. S. Department of Health, Education and Welfare, Public Health Service, Center for Disease Control, NIOSH, Rockville, Maryland.

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APPENDIX A

VOLATILE ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR AT VARIOUS GEOGRAPHICAL LOCATIONS WITHIN THE CONTINENTAL UNITED STATES

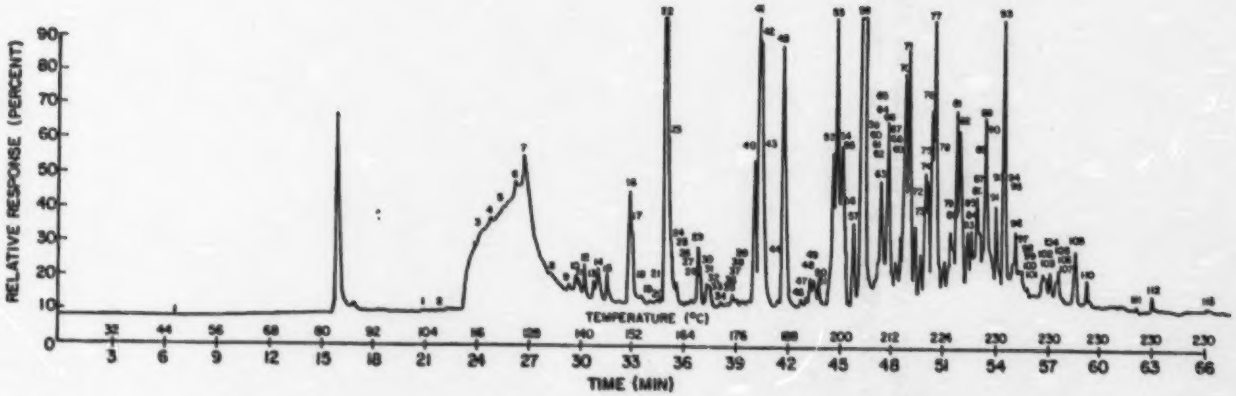

Figure 32. Profile of ambient air pollutants for South Charleston, WV using high resolution gas chromatography/mass spectrometry/computer. A 400 ft S.S. SCOT coated with OV-101 stationary phase and a temperature program of 20-230°C @ 4°C/min were used. See Table 38 for listing.

Table 38. ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR IN SOUTH CHARLESTON, WV[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1A	83	CO_2
1B	89	cyclopropane
1C	92	chloromethane
1D	95	1-butene
2	102	isopentane
2A	103	C_5H_{10} isomer
3	106	furan
3A	106	n-pentane
4	108	acetaldehyde
4A	109	C_5H_8 isomer
4B	110	C_5H_{10} isomer
4C	111	dichloromethane
5A	112	carbon disulfide
5	113	propanal
5B	114	methylsilane (BKG)
6	115-7	acetone
6A	116	C_6H_{12} isomer
6B	116	C_6H_{14} isomer
7	117	C_4H_8O isomer
8	120	C_6H_{14} isomer
9	124	n-hexane and 2-methylfuran
9A	125	C_6H_{12} isomer
10	126	3-methylfuran (tent.)
10A	128	trichloromethane
10B	129	methylcyclopentane
11	135	1,1,1-trichloroethane
11A	135	2-butanone
12	136	3,3-dimethylpentane
12A	137	benzene
12B	137	carbon tetrachloride
13	138	cyclohexane and C_7H_{16} isomer

(continued)

Table 38 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
14	139	2,3-dimethylpentane
15	140	C_7H_{14} isomer
16	141	3-methylhexane
17	142	C_7H_{14} isomer and C_7H_{16} isomer
18	143	dimethylcyclopentane isomer
20	145	_n_-heptane
20A	146	2,5-dimethylfuran (tent.)
20B	147	C_7H_{14} isomer
20C	148	2,4-dimethylfuran
21	149	2,2,4-trimethylpentane
22	150-2	methylcyclohexane
23	152	C_8H_{16} isomer
23A	153	2,4-dimethylhexane
24	154	ethylcyclopentane
25	156	trimethylcyclopentane isomer
25A	156	dimethyl disulfide
26	157	trimethylcyclopentane isomer
26A	158	C_9H_{18} isomer
27	159	2,3-dimethylhexane
28	160	toluene
29	161	3-methylheptane
30	164-5	dimethylcyclohexane isomer and 4-methyl-2-pentanone
31	166	1-octene
32	167	_n_-octane
33	169	hexamethylcyclotrisiloxane (BKG)
34	170	tetrachloroethylene
35	172	3-hexanone and isobutyl acetate
35A	172	C_8H_{14} isomer
36	174	C_9H_{20} isomer
36A	174	C_9H_{20} isomer
37	175	2-hexanone and dimethylcyclohexane isomer

(continued)

Table 38 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
38	176	n-butyl acetate
39	178	chlorobenzene
40	179	C_9H_{20} isomer
41	180	ethylbenzene
42	181	p-xylene
42A	183	C_9H_{20} isomer
42B	183	phenyl acetylene
42C	184	C_9H_{18} isomer
42D	185	C_9H_{18} isomer
43	186	styrene
44	187	o-xylene and n-nonane
45	191	C_9H_{18} isomer
46	192	$C_{10}H_{22}$ isomer
47	193	isopropylbenzene
48	194	$C_{10}H_{22}$ isomer
49	195	C_3-alkylcyclohexane isomer
49A	196	$C_{10}H_{22}$ isomer
49B	197	$C_{10}H_{20}$ isomer
50	198	$C_{10}H_{22}$ isomer
51	199	n-propylbenzene
51A	199	$C_{10}H_{22}$ isomer
52	199-200	m-ethyltoluene
53	200.5	1,3,5-trimethylbenzene and silane compound
54	201	$C_{11}H_{24}$ isomer
56	203	p-ethyltoluene
56A	204	1-decene
57	205	n-decane
58	206	1,2,4-trimethylbenzene
59	207	$C_{11}H_{22}$ isomer
60	208	benzaldehyde
60A	208	$C_{11}H_{24}$ isomer

(continued)

Table 38 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
61	209	m-dichlorobenzene or (p)
62	210	$C_{11}H_{24}$ isomer
63	210	C_4-alkyl benzene isomer
64	212	1,2,3-trimethylbenzene
65	213	$C_{11}H_{24}$ isomer
66	214	C_4-alkylcyclohexane isomer
67	215	α-methylstyrene
68	215	C_4-alkyl benzene isomer
69	216	C_4-alkyl benzene isomer
70	217	C_4-alkyl benzene isomer
71	218	$C_{11}H_{24}$ isomer
72	219	C_4-alkyl benzene isomer
73	220	C_4-alkyl benzene isomer
74	221	$C_{11}H_{22}$ isomer
74A	221	C_4-alkyl benzene isomer
75	222	n-undecane
76	223	dimethylstyrene isomer
76A	223	C_4-alkyl benzene isomer and $C_{12}H_{26}$ isomer
77	224	C_5-alkyl benzene and $C_{11}H_{22}$ isomers
	225	$C_{12}H_{26}$ isomer
78	225	$C_{12}H_{26}$ isomer
79	226	C_5-alkyl benzene isomer
81	227	C_4-alkyl benzene isomer
	228	silane compound and $C_{12}H_{26}$ isomer
82	228	$C_{12}H_{24}$ isomer
83	230	$C_{13}H_{28}$ isomer and C_5-alkyl benzene isomer
84	230	C_5-cyclohexane isomer
85	230	$C_{12}H_{26}$ isomer

(continued)

Table 38 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
86	230	$C_{12}H_{26}$ isomer
87	230	$C_{12}H_{26}$ isomer
88	230	silane compound (BKG)
89	230	$C_{13}H_{28}$ isomer
90	230	$C_{13}H_{28}$ isomer
91	230	n-dodecane
92	230	$C_{13}H_{28}$ isomer
	230	naphthalene

[a] Sampling site was 167 11th Ave. at the Dept. of Health, State Hygenic Laboratory. See Table 28 (S1) for sampling protocol.

Table 39. ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR IN S. CHARLESTON, WV[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	81	CO_2
2	88	1-butene
2A	89	n-butane
3	91	2-butene
4	101	isopentane
5	105	C_5H_{10} isomer and furan
5A	106	n-pentane
6	107	acetaldehyde
6A	108	dichloromethane
6B	109	cagbon disulfide (tent.)
7	111	propanal
7A	112	methylsilane
8	115	acetone
9	116	2-methylpentane
10	119	3-methylpentane
10A	121	C_6H_{12} isomer
11	123	n-hexane and 2-methylfuran
12	124	C_6H_{12} isomer
13	125	3-methylfuran and chloroform
14	128	C_6H_{14} isomer
14A	129	silane compound (BKG)
14B	130	2,2-dimethylpentane
15	131	2,4-dimethylpentane
15A	132	2,2,3-trimethylbutane
16	133	1,1,1-trichloroethane
16A	134	C_7H_{14} isomer and methyl ethyl ketone
16B	134	3,3-dimethylpentane
17	135	benzene
18	136	carbon tetrachloride
18A	136	cyclohexane
19	137	2-methylhexane

(continued)

Table 39 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
20	138	2,3-dimethylpentane
20A	139	C_7H_{14} isomer
21	140	3-methylhexane
21A	141	C_7H_{14} isomer
22	142	1,cis-2-dimethylcyclohexane
23	143	1,trans-2-dimethylcyclohexane
23A	144	C_7H_{14} + C_7H_{12} isomer
24	145	*n*-heptane
25	149	C_8H_{18} isomer
25A	150	dimethylcyclopentane isomer
26	150	methylcyclohexane
27	152	C_8H_{16} isomer
28	152	2,4-dimethylhexane
29	153	C_8H_{18} + C_8H_{16} isomer
29A	154	C_8H_{18} isomer
30	155	C_8H_{18} isomer
31	156	methylethylpentane isomer + C_8H_{16}
32	157	1,trans-2,cis-3-trimethylcyclopentane
33	157	C_8H_{18} isomer
34	158	2,3-dimethylhexane
35	159	toluene
36	161	3-methylheptane
37	164	4-methyl-2-pentanone + dimethylcyclohexane isomer
38	167	*n*-octane
39	169	hexamethylcyclotrisiloxane
40	170	tetrachloroethylene
41	172	isobutyl acetate
42	173	C_9H_{20} isomer
43	175	C_9H_{20} isomer
44	176	2-hexanone

(continued)

Table 39 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
45	177	n-butyl acetate
45A	178	chlorobenzene
46	179	C_9H_{20} isomer
47	180	ethylbenzene
48	181-4	p-xylene
48A	184	phenyl acetylene
49	185	dibutyl ether
50	186	styrene
51	189	o-xylene + n-nonane
52	191	$C_{10}H_{22}$ isomer
52A	191	C_9H_{18} isomer
53	192	$C_{10}H_{22}$ isomer
54	193	isopropylbenzene
55	194	$C_{10}H_{22}$ isomer
55A	194	$C_{10}H_{20}$ isomer
56	195	C_3-alkylcyclohexane isomer
57	196	$C_{10}H_{16}$ + $C_{10}H_{22}$ isomer
57A	197	$C_{10}H_{20}$ isomer
58A	197	$C_{10}H_{22}$ isomer
58	198	5-methylnonane
59	198	n-propylbenzene
60	199	m-ethyltoluene
61	200	3-methylnonane
62	201	1,3,5-trimethylbenzene
63	201	$C_{11}H_{24}$ isomer
64	201	$C_{10}H_{22}$ + silane compound
65	202	$C_{10}H_{22}$ isomer
66	203	o-ethyltoluene
66A	204	$C_{10}H_{20}$ isomer
67	205	n-decane
68	205	1,2,4-trimethylbenzene
	206	$C_{11}H_{22}$ isomer

(continued)

Table 39 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
69	208	$C_{10}H_{20}$ isomer
70	209	benzaldehyde + $C_{11}H_{24}$ isomer
71	209	isobutylbenzene
71A	210	$C_{11}H_{24}$ isomer
72	210	m- or p-dichlorobenzene
73	211	$C_{11}H_{24}$ isomer
73A	211	o-cymene
74	212	1,2,3-trimethylbenzene
75	213	$C_{11}H_{24}$ isomer
75A	213	$C_{11}H_{22}$ isomer
76	214	C_4-alkyl cyclohexane isomer
77	215	α-methylstyrene
77A	215	p-cymene
78	216	p-propyltoluene
79	216	$C_{11}H_{24}$ isomer
80	217	o-diethylbenzene
81	217	n-butylbenzene
82	218	$C_{12}H_{26}$ isomer
83	219	o-propyltoluene
83A	220	$C_{10}H_{18}$ isomer
84	220	dimethylethylbenzene isomer
85	221	n-undecane
86	222	$C_{12}H_{26}$ isomer
87	223	$C_{12}H_{26}$
88	225	C_5-alkyl benzene isomer
89	226	$C_{12}H_{26}$ isomer
90	227	$C_{12}H_{26}$ isomer
91	227	C_4-alkyl benzene isomer
92	229	$C_{12}H_{24}$ + $C_{11}H_{20}$ isomer
93	230	C_5-alkyl benzene isomer
94	230	C_4-alkyl benzene isomer
95	230	$C_{12}H_{26}$ isomer

(continued)

Table 39 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
96	230	$C_{12}H_{26}$ isomer
97	230	$C_{13}H_{28}$ isomer
98	230	silane compound (BKG)
100	230	$C_{13}H_{28}$ isomer
101	230	$C_{13}H_{28}$ isomer
102	230	$C_{12}H_{24}$ isomer
103	230	*n*-dodecane

[a] See Table 28 (S2) for sampling protocol.

Table 40. POLLUTANTS IDENTIFIED IN AMBIENT AIR FROM SOUTH CHARLESTON, WV[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	85	carbon dioxide
2	88	chloromethane (tent.)
3	89	ethylene oxide (tent.)
4	91	2-methylpropene (tent.)
5	97	chloroethane (tent.)
6	100	C_5H_{12}
7	101	trichlorofluoromethane (tent.)
8	104	ethanol
9	109	propylene oxide (tent.)
10	113	acetone
11	115	C_6H_{14}
12	117	2-propanol (tent.)
13	119	C_6H_{14}
14	121	C_6H_{14}
14A	121	2-methylpropenal (tent.)
15	123	vinyl acetate
16	124	2-methylfuran
17	130	methyl vinyl ketone
18	132	methyl ethyl ketone
19	133	3,3-dimethylpentane
20	134	benzene
21	135	carbon tetrachloride
22	135	cyclohexane
23	136	C_7H_{16}
24	136	C_7H_{16}
25	138	C_7H_{16}
26	140	C_7H_{14}
27	141	C_7H_{14}
28	143	C_7H_{16}
29	148	C_7H_{14}

(continued)

Table 40 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
30	148	C_7H_{14}
31	152	C_8H_{18}
32	152	C_7H_{14}
33	154	C_8H_{16}
34	155	C_8H_{16}
35	156	C_8H_{18}
36	158	toluene
37	160	C_8H_{18}
38	163	C_8H_{16}
39	164	C_8H_{16}
40	165	C_8H_{18}
41	167	dibromodichloromethane (tent.)
42	168	hexamethylcyclotrisiloxane
43	168	tetrachloroethylene
44	172	C_8H_{16}
45	175	chlorobenzene
46	177	C_9H_{20}
47	178	ethylbenzene
48	179	_p_-xylene
49	180	_m_-xylene
50	182	phenylacetylene
51	184	C_9H_{18}
52	185	_o_-xylene
52A	185	C_9H_{20}
53	191	C_9H_{20}
54	192	isopropylbenzene
55	193	C_9H_{20}
56	194	C_9H_{18}
57	196	C_9H_{18}
58	197	_n_-propylbenzene
59	198	_m_-ethyltoluene

(continued)

Table 40 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
60	198	p-ethyltoluene
61	199	1,3,5-trimethylbenzene
62	199	unknown m/e 133, 193, 191, 249, 251
63	200	$C_{10}H_{22}$
64	202	o-ethyltoluene
65	202	$C_{10}H_{20}$
66	203	$C_{10}H_{22}$
67	203	1,2,4-trimethylbenzene
68	206	benzaldehyde
69	207	C_4-alkyl benzene
70	208	m-dichlorobenzene
71	208	C_4-alkyl benzene
72	209	1,2,3-trimethylbenzene
73	211	acetophenone
73A	211	p-dichlorobenzene
74	212	$C_{10}H_{20}$
75	212	C_4-alkyl benzene
76	212	indan
77	213	C_4-alkyl benzene
78	213	o-dichlorobenzene
79	213	C_4-alkyl benzene
80	214	C_4-alkyl benzene
81	215	C_4-alkyl benzene
82	215	$C_{11}H_{24}$
83	216	$C_{11}H_{24}$
84	217	C_4-alkyl benzene
85	218	C_4-alkyl benzene
86	218	C_4-alkyl benzene
87	219	C_4-alkyl benzene
88	220	$C_{11}H_{24}$

(continued)

Table 40 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
89	221	methylindan (tent.)
90	221	C_4-alkyl benzene
91	222	C_5-alkyl benzene
92	223	C_5-alkyl benzene
93	224	C_4-alkyl benzene
94	224	C_5-alkyl benzene
95	225	$C_{12}H_{26}$
96	225	C_4-alkyl benzene
97	226	C_4-alkyl benzene
98	226	unknown, m/e 73
99	228	C_5-alkyl benzene
100	229	C_5-alkyl benzene
101	229	$C_{12}H_{26}$
102	230	methylindan (tent.)
103	230	unknown, m/e 105, 106
104	230	$C_{12}H_{26}$
105	230	C_5-alkyl benzene
106	230	methylindan (tent.)
107	230	C_5-alkyl benzene
108	230	$C_{12}H_{26}$
109	230	C_5-alkyl benzene
110	230	C_5-alkyl benzene
111	230	tetralin
112	230	C_5-alkyl benzene
113	230	C_5-alkyl benzene
113A	230	$C_{12}H_{26}$
114	230	$C_{12}H_{26}$
115	230	$C_{12}H_{24}$
116	230	C_5H_9-alkyl benzene
117		C_5-alkyl benzene
118		$C_{12}H_{26}$

(continued)

Table 40 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
119		naphthalene
120		C_5-alkyl benzene
121		unknown alkane
122		C_6-alkyl benzene
123		C_6-alkyl benzene
124		unknown
125		unknown
126		$C_{13}H_{26}$
127		$C_{13}H_{28}$
128		$C_{13}H_{26}$
129		$C_{13}H_{28}$
130		$C_{13}H_{28}$
131		$C_{13}H_{28}$
132		$C_{14}H_{30}$
133		C_6-alkyl benzene
134		C_6-alkyl benzene
135		$C_{13}H_{28}$
136		$C_{14}H_{28}$ (tent.)
137		$C_{14}H_{30}$ (tent.)
138		unknown, m/e 73
139		$C_{14}H_{30}$
140		$C_{13}H_{26}$ (tent.)
141		unknown
142		2-methylnaphthalene
143		$C_{14}H_{28}$ (tent.)
144		$C_{14}H_{28}$ (tent.)
145		$C_{14}H_{30}$ (tent.)
146		1-methylnaphthalene
147		$C_{14}H_{30}$ (tent.)
148		$C_{14}H_{30}$ (tent.)
149		$C_{15}H_{32}$

(continued)

Table 40 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
150		$C_{14}H_{28}$ (tent.)
151		$C_{14}H_{30}$
152		$C_{14}H_{30}$ (tent.)
153		unknown
154		unknown, m/e 73
155		$C_{15}H_{32}$
156		unknown

[a] See Table 28 (S9) for sampling protocol.

Table 41. POLLUTANTS IDENTIFIED IN AMBIENT AIR IN C. H. MILBY PARK, PASADENA, TX[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	32	2-methylpropene
2	33	C_4H_8 isomer
3	34	chloroethane
4	38	furan
5	39	methylene chloride
6	41	acetone
7	43	C_6H_{14} isomer
8	47	isopropanol
9	48	chloroform
9A	49	2-chloro-1,3-butadiene
9B	49	1-chlorobutene-3-yne
10	51	C_6H_{14} isomer
11	52	C_6H_{12} isomer
12	53	methyl ethyl ketone
13	55	benzene
13A	55	carbon tetrachloride
14	56	cyclohexane
15	57	C_7H_{16} isomer
16	57	C_7H_{16} isomer
17	58	C_7H_{14} isomer
18	60	C_7H_{14} isomer
19	62	C_7H_{14} isomer
20	64	_n_-heptane
21	66	dimethylfuran isomer
22	68	C_7H_{14} isomer
23	70	C_8H_{18} isomer
24	72	C_8H_{16} isomer
25	73	C_8H_{16} isomer
26	76	toluene
27	77	C_8H_{18} isomer
28	78	C_8H_{18} isomer
29	79	C_6H_{16} isomer

(continued)

Table 41 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
30	82	C_8H_{18} isomer
31	84	n-octane
32	89	C_9H_{20} isomer
33	90	4-vinylcyclohexene
34	92	chlorobenzene
35	95	ethyl benzene
36	98	p-xylene
37	99	m-xylene
37A	99	phenyl acetylene
38	102	styrene
38A	102	cyclooctatetraene
39	105	o-xylene
39A	105	n-nonane
40	106	C_9H_{18} isomer
41	108	cumene
42	110	C_9H_{18} isomer
43	112	$C_{10}H_{16}$ isomer
44	114	n-propylbenzene
45	115	benzaldehyde
46	116	C_3-alkyl benzene
47	118	C_3-alkyl benzene
48	120	$C_{10}H_{20}$ isomer
49	122	C_3-alkyl benzene
50	124	n-decane
50A	124	m-dichlorobenzene
51	126	C_4-alkyl benzene
52	127	$C_{10}H_{18}$ isomer
53	128	o-dichlorobenzene
54	130	$C_{11}H_{24}$ isomer
55	131	C_4-alkyl benzene
56	132	C_4-alkyl benzene
57	134	C_4-alkyl benzene

(continued)

Table 41 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
58	134	C_4-alkyl benzene
59	136	$C_{10}H_{12}$ isomer
60	137	$C_{10}H_{12}$ isomer
61	139	$C_{11}H_{22}$ isomer
62	140	n-undecane
63	142	C_5-alkyl benzene
64	144	C_4-alkyl benzene
65	144	$C_{12}H_{26}$ isomer
66	145	C_5-alkyl benzene
67	147	$C_{10}H_{12}$ isomer
68	148	C_5-alkyl benzene
69	149	$C_{12}H_{26}$ isomer
70	150	$C_{13}H_{28}$ isomer
71	151	C_5-alkyl benzene
72	152	$C_{13}H_{28}$ isomer
73	153	naphthalene
74	155	$C_{13}H_{26}$ isomer
75	156	n-dodecane
76	157	$C_{13}H_{28}$ isomer
77	159	$C_{13}H_{28}$ isomer
78	161	$C_{13}H_{26}$ isomer
79	163	$C_{13}H_{26}$ isomer
80	164	$C_{13}H_{28}$ isomer
81	166	$C_{13}H_{28}$ isomer
82	167	$C_{13}H_{26}$ isomer
83	168	$C_{14}H_{30}$ isomer
84	173	n-tridecane
85	174	$C_{14}H_{28}$ isomer
86	176	$C_{15}H_{32}$ isomer
87	178	$C_{15}H_{32}$ isomer
88	180	$C_{15}H_{32}$ isomer

(continued)

Table 41 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
89	182	$C_{15}H_{32}$ isomer
90	183	$C_{14}H_{28}$ isomer
91	185	_n_-tetradecane
92	194	$C_{15}H_{32}$ isomer
93	198	_n_-pentadecane
94	199	$C_{15}H_{30}$ isomer
95	210	_n_-hexadecane

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[a] Pollutants were resoled on a 42 m glass SCOT capillary coated with OV-101 stationary phase programmed from 20-220°C @ 4°/min. Carrier (He) gas was ∿1.5 ml/min. Sampling protocol is given in Table 29 (S1).

Table 42. POLLUTANTS IDENTIFIED IN AMBIENT AIR IN C. H. MILBY PARK, PASADENA, TX[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	79	methyl chloride
2	80	n-propane
3	85	C_4H_6 isomer
4	88	isopentane
5	91	trichlorofluoromethane
6	92	chlorofluoromethane
7	94	acetaldehyde
7A	95	furan
8	96	methylene chloride
9	96	carbon disulfide
10	100	acetone
11	104	isopropanol
12	108	3-methylpentane
13	110	2-methylfuran
14	113	chloroform
15	115	2-chloro-1,3-butadiene
15A	115	1-chlorobutene-3-yne
16	116	C_7H_{16} isomer
16A	116	C_6H_{12} isomer
17	118	methyl ethyl ketone
18	119	1,1,1-trichloroethane
19	121	C_6H_{10} isomer
20	123	benzene
20A	123	carbon tetrachloride
21	124	cyclohexane
22	125	C_7H_{16} isomer
23	126	C_7H_{16} isomer
24	127	C_7H_{16} isomer
25	129	C_7H_{14} isomer
26	130	C_8H_{18} isomer
27	132	n-heptane

(continued)

Table 42 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
28	136	dimethylfuran isomer
29	137	C_8H_{18} isomer
30	138	C_7H_{14} isomer
31	140	C_8H_{18} isomer
32	141	C_8H_{18} isomer
33	142	C_8H_{16} isomer
34	144	C_8H_{16} isomer
35	144	C_8H_{16} isomer
36	145	C_8H_{16} isomer
37	146	toluene
38	147	C_8H_{18} isomer
39	148	C_8H_{18} isomer
40	149	C_8H_{16} isomer
41	151	C_8H_{16} isomer
42	152	$C_6H_{12}O$ isomer
43	152	C_8H_{18} isomer
44	154	n-octane
45	156	tetrachloroethylene
46	157	C_8H_{16} isomer
47	160	C_9H_{20} isomer
48	161	C_9H_{20} isomer
49	162	4-vinylcyclohexene
50	163	C_9H_{18} isomer
51	165	chlorobenzene
52	166	ethylbenzene
53	168	p-xylene
54	169	m-xylene
55	170	phenyl acetylene
56	171	styrene
57	173	C_9H_{20} isomer
58	174	o-xylene
58A	174	n-nonane

(continued)

Table 42 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
59	176	C_9H_{18} isomer
60	178	1,4-dichloro-2-butene (tent.)
61	180	cumene
62	180	$C_{10}H_{16}$ isomer
63	181	2-furaldehyde
64	182	α-pinene
65	184	$C_{10}H_{20}$ isomer
66	184	$C_{10}H_{22}$ isomer
67	185	n-propylbenzene
68	186	m-ethyltoluene
69	186	p-ethyltoluene
70	187	benzaldehyde
71	188	C_3-alkyl benzene
72	190	C_3-alkyl benzene
73	191	$C_{10}H_{20}$ isomer
74	192	n-decane
74A	192	o-ethyltoluene
75	195	$C_{10}H_{20}$ isomer
76	196	m-dichlorobenzene
77	196	$C_{11}H_{24}$ isomer
78	197	C_3-alkyl benzene
79	198	C_4-alkyl benzene
80	200	$C_{11}H_{24}$ isomer
81	201	C_9H_{10} isomer
82	202	C_9H_{10} isomer
83	203	o-dichlorobenzene
84	203	C_4-alkyl benzene
85	204	$C_{11}H_{24}$ isomer
86	204	C_4-alkyl benzene
87	205	$C_{11}H_{24}$ isomer
88	206	C_4-alkyl benzene

(continued)

Table 42 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
89	207	C_4-alkyl benzene
90	208	$C_{12}H_{24}$ isomer
91	209	C_4-alkyl benzene
92	210	_n_-undecane
93	211	acetophenone
94	212	C_5-alkyl benzene
95	213	C_5-alkyl benzene
96	214	C_5-alkyl benzene
97	215	C_4-alkyl benzene
98	215	C_4-alkyl benzene
99	216	C_6-alkyl benzene
100	217	C_5-alkyl benzene
101	218	C_5-alkyl benzene
102	219	$C_{10}H_{11}$ isomer
103	220	C_5-alkyl benzene
104	220	C_5-alkyl benzene
105	221	$C_{10}H_{11}$ isomer
106	222	C_5-alkyl benzene
107	224	C_5-alkyl benzene
108	225	$C_{12}H_{24}$ isomer
109	226	_n_-dodecane
110	227	1,3,5-trichlorobenzene
111	228	naphthalene
112	229	$C_{13}H_{28}$ isomer
113	230	$C_{13}H_{28}$ isomer
114	231	C_6-alkyl benzene
115	232	$C_{13}H_{26}$ isomer
116	234	$C_{12}H_{24}$ isomer
117	235	C_6-alkyl benzene
118	236	$C_{13}H_{26}$ isomer
119	237	$C_{11}H_{14}$ isomer
120	238	$C_{14}H_{30}$ isomer

(continued)

Table 42 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
121	239	$C_{13}H_{26}$ isomer
122	240	n-tridecane
123	240	$C_{14}H_{28}$ isomer
124	isothermal	$C_{14}H_{30}$ isomer
125	isothermal	β-methylnaphthalene
126	isothermal	$C_{14}H_{30}$ isomer
127	isothermal	$C_{14}H_{28}$ isomer
128	isothermal	α-methylnaphthalene
129	isothermal	$C_{14}H_{30}$ isomer
130	isothermal	$C_{14}H_{30}$ isomer
131	isothermal	$C_{14}H_{30}$ isomer
132	isothermal	$C_{15}H_{32}$ isomer
133	isothermal	$C_{14}H_{28}$ isomer
134	isothermal	n-tetradecane
135	isothermal	biphenyl
136	isothermal	$C_{15}H_{32}$ isomer
137	isothermal	phenyl ether
138	isothermal	$C_{15}H_{32}$ isomer
139	isothermal	$C_{15}H_{30}$ isomer
140	isothermal	$C_{15}H_{32}$ isomer
141	isothermal	$C_{14}H_{28}$ isomer
142	isothermal	$C_{15}H_{32}$ isomer
143	isothermal	$C_{15}H_{30}$ isomer
144	isothermal	n-pentadecane
145	isothermal	$C_{15}H_{30}$ isomer
146	isothermal	n-hexadecane

[a] A 400 ft stainless steel SCOT capillary coated with OV-101 was used for resolving pollutants. Capillary was programmed from 20-240°C @ 4°C/min Carrier (He) was ~3.0 ml/min. Sampling protocol is given in Table 29 (S1, duplicate sample).

Table 43. POLLUTANTS IDENTIFIED IN AMBIENT AIR FROM PASADENA, TX[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	72	propylene
1A	72	propane
2	75	chloromethane
3	77	butene isomer
4	78	n-butane
5	86	C_5H_{12} isomer
6	88	chlorofluoromethane
7	90	C_5H_{12} isomer
8	92	methylene chloride
9	94	carbon disulfide
10	96	propanal (tent.)
11	98	acetone
12	100	C_6H_{14} isomer
13	103	3-methyl pentane
14	105	C_6H_{12} isomer
15	107	C_6H_{14} isomer
15A	107	2-methylfuran
16	108	C_6H_{12} isomer
17	109	C_5H_{10}
17A	110	methyl isopropyl ketone (tent.)
18	113	methylcyclopentane
19	114	C_7H_{16} isomer
20	118	1,2-dichloroethane
21	120	benzene
22	121	cyclohexane
23	122	C_7H_{16} isomer
24	123	C_7H_{16} isomer
25	124	C_7H_{16} isomer
26	126	dimethylcyclopentane isomer
27	127	dimethylcyclopentane isomer
28	128	trichloroethylene

(continued)

Table 43 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
29	129	n-heptane
29A	130	C_7H_{14} isomer
30	132	dimethylfuran
30A	132	m/e 94
31	133	dimethylfuran isomer
32	136	dimethylpentene isomer
33	137	C_7H_{14} isomer
34	138	C_8H_{16} isomer
35	140	methylmethacrylate (tent.)
36	142	C_8H_{16} isomer
37	143	C_8H_{16} isomer
38	143	C_8H_{18} isomer
39	144	toluene
40	146	C_8H_{18} isomer
41	148	C_8H_{16} isomer
42	150	C_8H_{16} isomer
43	150	C_9H_{20} isomer
44	151	n-octane
45	153	C_8H_{16} isomer
45A	153	dibromodichloromethane
46	154	tetrachloroethylene
47	156	C_8H_{16} isomer
48	158	C_8H_{16} isomer
49	159	C_9H_{20} isomer
50	160	C_9H_{20} isomer
51	161	C_8H_{16} isomer
51A	161	C_9H_{18} isomer
52	163	chlorobenzene
53	164	C_9H_{20} isomer
54	164	C_9H_{20} isomer
55	165	ethylbenzene

(continued)

Table 43 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
56	166	p-xylene
57	167	m-xylene
58	168	phenylacetylene
58A	170	C_9H_{18} isomer
59	170	bromoform
60	171	styrene
61	171	o-xylene
62	172	n-nonane
63	174	C_9H_{18} isomer
64	176	C_9H_{18} isomer
65	177	$C_{10}H_{22}$ isomer
66	178	isopropylbenzene
67	179	$C_{10}H_{20}$ isomer
68	180	$C_{10}H_{22}$ isomer
69	182	n-propylcyclohexane
70	182	$C_{10}H_{16}$ isomer
70A	183	cyclohexanone (tent.)
71	183	$C_{10}H_{20}$ isomer
72	184	$C_{10}H_{22}$ isomer
73	184	n-propylbenzene
74	185	m-ethyltoluene
74A	185	p-ethyltoluene
75	186	o-ethyltoluene
75A	186	$C_{11}H_{24}$ isomer
76	188	$C_{10}H_{20}$ isomer
77	189	1,3,5-trimethylbenzene
78	190	$C_{10}H_{20}$ isomer
79	191	C_9H_{10} isomer
80	192	1,2,4-trimethylbenzene
80A	192	n-decane
81	193	C_9H_{10} isomer

(continued)

Table 43 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
81A	193	benzaldehyde
82	195	isobutylbenzene
83	195	sec-butylbenzene
83A	195	m-dichlorobenzene
83B	195	$C_{11}H_{24}$ isomer
84	196	$C_{11}H_{24}$ isomer
85	197	1,2,3-trimethylbenzene
86	198	$C_{10}H_{16}$ isomer
87	199	$C_{11}H_{24}$ isomer
88	200	n-butylcyclohexane
89	200	C_9H_{10} isomer
89A	200	o-dichlorobenzene
90	202	C_4-alkyl benzene
91	202	C_4-alkyl benzene
92	203	C_4-alkyl benzene
93	203	C_4-alkyl benzene
94	204	C_4-alkyl benzene
95	205	C_4-alkyl benzene
95A	205	$C_{10}H_{18}$ isomer
96	207	C_4-alkyl benzene
97	207	C_4-alkyl benzene
98	208	C_4-alkyl benzene
98A	208	$C_{10}H_{12}$ isomer
99	209	n-undecane
100	211	C_5-alkyl benzene
100A	211	$C_{11}H_{22}$ isomer
101	212	C_4-alkyl benzene
102	214	$C_{12}H_{24}$ isomer
103	214	C_4-alkyl benzene
104	214	$C_8H_{11}N$ isomer
105	215	m/e 152

(continued)

Table 43 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
106	216	$C_{12}H_{26}$ isomer
107	217	C_5-alkyl benzene
108	218	$C_{11}H_{22}$ isomer
109	218	C_5-alkyl benzene
110	219	C_5-alkyl benzene
111	220	$C_{12}H_{26}$ isomer
112	220	C_5-alkyl benzene
113	221	C_5-alkyl benzene
114	222	C_5-alkyl benzene
114A	222	$C_{11}H_{24}$ isomer
115	223	C_5-alkyl benzene
116	224	$C_{12}H_{24}$ isomer
116A	224	C_6-alkyl benzene
117	226	n-dodecane
118	226	C_5-alkyl benzene
119	227	naphthalene
120	228	$C_{11}H_{14}$ isomer
120A	228	C_6-alkyl benzene
121	229	C_5-alkyl benzene
121A	229	C_6-alkyl benzene
122	230	C_6-alkyl benzene
123	230	$C_{13}H_{26}$ isomer
124	231	$C_{13}H_{26}$ isomer
125	232	C_6-alkyl benzene
126	233	$C_{13}H_{26}$ isomer
127	234	$C_{11}H_{24}$ isomer
128	234	C_6-alkyl benzene
129	235	$C_{13}H_{26}$ isomer
130	236	C_6-alkyl benzene
131	237	$C_{14}H_{30}$ isomer
132	238	$C_{13}H_{26}$ isomer

(continued)

Table 43 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
133	239	C_6-alkyl benzene
134	240	$C_{11}H_{14}$ isomer
135	240	n-tridecane
136	240	C_5-alkyl benzene
137	240	$C_{14}H_{28}$ isomer
138	240	$C_{14}H_{30}$ isomer
139	240	$C_{14}H_{28}$ isomer
140	240	$C_{14}H_{30}$ isomer
141	240	2-methylnaphthalene
142	240	$C_{14}H_{30}$ isomer
143	240	$C_{14}H_{30}$ isomer
144	240	$C_{14}H_{28}$ isomer
145	240	1-methylnaphthalene
146	240	$C_{14}H_{28}$ isomer
147	240	$C_{13}H_{26}$ isomer
148	240	$C_{14}H_{30}$ isomer
149	240	$C_{14}H_{30}$ isomer
150	240	$C_{15}H_{32}$ isomer
151	240	$C_{14}H_{30}$ isomer
152	240	n-tetradecane
153	240	m/e 154
154	240	$C_{15}H_{32}$ isomer
155	240	$C_{14}H_{28}$ isomer
156	240	$C_{15}H_{32}$ isomer
157	240	$C_{15}H_{30}$ isomer
158	240	$C_{15}H_{30}$ isomer
159	240	$C_{15}H_{32}$ isomer
160	240	$C_{15}H_{32}$ isomer
161	240	$C_{15}H_{32}$ isomer
162	240	$C_{15}H_{32}$ isomer

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[a] See Table 29 (S2) for sampling protocol.

Table 44. POLLUTANTS IDENTIFIED IN AMBIENT AIR FROM PASADENA, TX[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	74	propane
2	78	chloromethane
2A	79	isobutane
3	81	butene isomer
4	82	_n_-butane
5	91	chloroethane
6	95	C_5H_{12} isomer
7	97	chlorofluoromethane (tent.)
7A	98	_n_-pentane
8	102	propanal (tent.)
9	105	acetone
10	110	C_6H_{14} isomer
11	113	_n_-hexane
12	116	chloroform
13	119	methylcyclopentane
14	120	C_7H_{16}
14A	120	1,2-dichloroethane
15	124	benzene
16	126	carbon tetrachloride
17	126	cyclohexane
18	127	C_7H_{16} isomer
19	128	C_7H_{16} isomer
20	130	C_7H_{16} isomer
21	132	dimethylcyclopentane isomer
22	133	dimethylcyclopentane isomer
23	135	_n_-heptane
24	136	dimethylfuran isomer
25	138	dimethylfuran isomer
26	139	C_8H_{18} isomer
27	140	dimethylpentene isomer

(continued)

Table 44 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
28	141	C_8H_{18} isomer
29	142	C_8H_{16} isomer
30	144	C_8H_{16} isomer
31	146	C_8H_{18} isomer
32	147	C_8H_{18} isomer
33	148	toluene
34	150	C_8H_{18} isomer
35	152	C_8H_{16} isomer
36	152	$C_6H_{12}O$ (aldehyde ?)
37	153	C_8H_{18} isomer
38	154	C_8H_{18} isomer
39	155	_n_-octane
39A	157	dibromodichloromethane (tent.)
40	158	tetrachloroethylene
41	159	C_8H_{16} isomer
42	160	C_9H_{20} isomer
43	162	C_9H_{20} isomer
44	163	C_8H_{16} isomer
45	163	C_8H_{16} isomer
46	164	C_9H_{20} isomer
47	165	chlorobenzene
48	166	C_9H_{20} isomer
49	167	ethylbenzene
50	168	_p_-xylene
51	169	_m_-xylene
52	170	phenylacetylene
52A	171	bromoform
53	173	styrene
54	174	_o_-xylene
55	175	_n_-nonane
55A	176	C_9H_{18} isomer

(continued)

Table 44 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
56	179	$C_{10}H_{22}$ isomer
57	180	$C_{10}H_{22}$ isomer
58	180	isopropylbenzene
59	181	C_9H_{18} isomer
60	182	$C_{10}H_{16}$ isomer
61	183	$C_{10}H_{20}$ isomer
62	184	$C_{10}H_{22}$ isomer
63	185	_n_-propylbenzene
64	186	_m_-ethyltoluene
65	186	_p_-ethyltoluene
66	187	_o_-ethyltoluene
67	189	$C_{11}H_{24}$ isomer
68	190	1,3,5-trimethylbenzene
69	191	$C_{10}H_{20}$ isomer
70	192	$C_{10}H_{20}$ isomer
70A	192	1,2,4-trimethylbenzene
71	193	_n_-decane
71A	193	benzaldehyde
72	194	C_9H_{10} isomer
73	195	$C_{10}H_{20}$ isomer
74	196	C_5-alkyl benzene
75	196	_m_-dichlorobenzene
76	197	$C_{11}H_{24}$ isomer
77	198	C_4-alkyl benzene
78	199	1,2,3-trimethylbenzene
78A	199	$C_{10}H_{12}$ isomer
79	200	$C_{10}H_{16}$ isomer
80	200	$C_{10}H_{16}$ isomer
81	201	$C_{10}H_{20}$ isomer
82	201	C_9H_{10} isomer
83	202	$C_{11}H_{22}$ isomer

(continued)

Table 44 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
83A	202	o-dichlorobenzene
84	203	C_4-alkyl benzene
85	203	C_4-alkyl benzene
86	204	C_4-alkyl benzene
87	205	$C_{10}H_{20}$ isomer
88	206	C_4-alkyl benzene
89	207	C_4-alkyl benzene
90	208	C_4-alkyl benzene
91	209	C_4-alkyl benzene
92	209	n-undecane
93	210	C_5-alkyl benzene
94	211	$C_{11}H_{22}$ isomer
95	213	C_5-alkyl benzene
96	214	$C_{11}H_{22}$ isomer
97	214	C_4-alkyl benzene
98	215	C_4-alkyl benzene
99	216	m/e 152
100	216	m/e 73 (Bkd ?)
101	217	C_5-alkyl benzene
102	218	$C_{11}H_{22}$ isomer
103	218	C_5-alkyl benzene
104	219	C_5-alkyl benzene
105	220	$C_{12}H_{26}$ isomer
106	221	C_5-alkyl benzene
107	221	C_5-alkyl benzene
108	222	C_5-alkyl benzene
109	223	C_5-alkyl benzene
110	224	$C_{12}H_{24}$ isomer
111	225	n-dodecane
112	226	$C_{11}H_{14}$ isomer
113	227	naphthalene

(continued)

Table 44 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
114	228	C_5-alkyl benzene
115	229	C_4-alkyl benzene
116	230	$C_{12}H_{22}$ isomer
117	230	C_5-alkyl benzene
117A	230	C_6-alkyl benzene
118	231	C_5-alkyl benzene
119	232	$C_{13}H_{26}$ isomer
120	232	$C_{13}H_{26}$ isomer
121	233	C_6-alkyl benzene
122	234	$C_{12}H_{24}$ isomer
123	234	C_6-alkyl benzene
124	235	$C_{13}H_{28}$ isomer
125	236	C_6-alkyl benzene
126	237	$C_{14}H_{30}$ isomer
127	238	C_6-alkyl benzene
128	239	$C_{14}H_{30}$ isomer
129	239	$C_{14}H_{28}$ isomer
130	240	n-tridecane
131	240	$C_{13}H_{26}$ isomer
132	240	$C_{13}H_{26}$ isomer
133	240	$C_{14}H_{28}$ isomer
134	240	$C_{14}H_{30}$ isomer
135	240	$C_{14}H_{30}$ isomer
136	240	2-methylnaphthalene
137	240	$C_{14}H_{30}$ isomer
138	240	1-methylnaphthalene
139	240	$C_{14}H_{30}$ isomer
140	240	$C_{14}H_{30}$ isomer
141	240	$C_{14}H_{30}$ isomer
142	240	$C_{15}H_{32}$ isomer
143	240	$C_{15}H_{32}$ isomer

(continued)

Table 44 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
144	240	$C_{15}H_{32}$ isomer
145	240	$C_{14}H_{30}$ isomer
146	240	$C_{14}H_{28}$ isomer
147	240	n-tetradecane
148	240	$C_{14}H_{28}$ isomer
149	240	biphenyl
150	240	$C_{14}H_{28}$ isomer
151	240	$C_{15}H_{32}$ isomer
152	240	$C_{15}H_{32}$ isomer
153	240	$C_{15}H_{30}$ isomer
154	240	$C_{14}H_{28}$ isomer
155	240	$C_{15}H_{32}$ isomer
156	240	$C_{16}H_{34}$ isomer
157	240	$C_{15}H_{32}$ isomer
158	240	$C_{16}H_{34}$ isomer
159	240	$C_{15}H_{30}$ isomer
160	240	$C_{15}H_{32}$ isomer
161	240	$C_{16}H_{34}$ isomer
162	240	n-pentadecane
163	240	$C_{15}H_{30}$ isomer
164	240	$C_{15}H_{30}$ isomer
165	240	$C_{16}H_{34}$ isomer

[a] See Table 29 (S3) for sampling protocol.

Table 45. POLLUTANTS IDENTIFIED IN NIGHT AMBIENT AIR IN PASADENA, TX[a]

Chromatographic Peak No.[a]	Elution Temperature (°C)	Compound
	73	CO_2
	74	ethylene oxide
2	81	propane
3	84	1-butene
3A	85	n-butane
4	94	isopentane
4A	95	acetaldehyde
4B	97	furan + C_5H_{10} isomer
5	98	n-pentane
5A	99	propionaldehyde
5B	100	C_5H_{10} isomer
5C	101	methylene chloride
5D	101	CS_2
7	105-110	acetone
9	113	2-methylpentane
10	114	3-methylpentane
10A	114	sec-butanol
10B	115	1-hexene
11	116	n-hexane
11A	117	C_6H_{10} + C_6H_{12} isomer
11B	118	chloroform
11C	119	C_6H_{12} isomer
11D	120	C_6H_{14} isomer
12	122	methylcyclopentane
12A	123	allyl acetate
12B	125	C_6H_{14} isomer
12C	127	C_6H_8 isomer
13	129	benzene
13A	129	CCl_4
13B	130	cyclohexane
14	130	2-methylhexane

(continued)

Table 45 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
15	131	2,3-dimethylpentane
16	132	3-methylhexane
17	133	C_7H_{12} isomer
17A	134	C_7H_{14} isomer
17B	134	C_7H_{16} isomer
17C	135	C_7H_{14} isomer
17D	135	1-trans-2-dimethylcyclopentane
18	137	_n_-heptane
18A	138	C_7H_{12} isomer
18B	139	C_7H_{14} isomer
18C	140	C_7H_{12} isomer
18D	141	trimethylpentane isomer
19	142	4,4-dimethyl-2-pentene
20	144	2,4-dimethylhexane
20A	144	cycloheptane
21	146	n-propylcyclopentane
22	148	2-methyl-trans-3-heptene
22A	148	2,3-dimethylhexane
23	149-150	toluene
24	150-151	2-methylheptane
25	152	3-methylheptane
26	154	trimethyl-2-pentene isomer
27	156-158	_n_-octane
27A	158	C_8H_{16} isomer
27B	158	hexamethylcyclotrisiloxane (BKG)
28	159	tetrachloroethylene
29	162	methyl isobutyl ketone
29A	163	3-methyl-3-ethyl-pentane
30	164	2,6-dimethylheptane
30A	164	C_9H_{20} isomer

(continued)

Table 45 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
31	165	ethylcyclohexane
32A	166	7-methyl-octene-1
32	167	chlorobenzene
33	169	ethylbenzene
34	170-171	p-xylene
35	171-172	phenylacetylene
36	175	styrene
37	175-176	o-xylene
38	176-178	n-nonane
39	180	methylethylcyclohexane isomer
39A	181	$C_{10}H_{22}$ isomer
40	182	isopropylbenzene
41	183	3-methylnonane
41A	183	$C_{10}H_{20}$ isomer
41B	184	propylcyclohexane
42	185	$C_{10}H_{16}$ isomer
43	186	$C_{10}H_{20}$ isomer
44	187	n-propylbenzene
45	188	p-ethyltoluene
46	188	C_3-alkyl benzene + $C_{10}H_{22}$ isomer
47	189	C_3-alkyl benzene
48	190	C_3-alkyl benzene + $C_{10}H_{22}$ isomer
49	192	1-methyl-4-isopropylcyclohexane
50	193-195	n-decane + o-ethyltoluene
51	195	benzaldehyde
51A	196	C_4-alkyl benzene isomer
52	197	dichlorobenzene isomer
53	198	methyldecane isomer and β-methylstyrene
54	198	o-cymene

(continued)

Table 45 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
55	199	$C_{11}H_{24}$ isomer
56	200	1,2,3-trimethylbenzene
57	201	$C_{11}H_{24}$ isomer
58	202	butylcyclohexane
58A	203	o-methylstyrene
58B	203	1,2-diethylbenzene
59	204	n-propyltoluene
60	205	p-diethylbenzene
61	205	methyldecane isomer
62	206	$C_{11}H_{24}$ isomer
63	207	o-propyltoluene
64	209	dimethylethylbenzene isomer
65	210	$C_{10}H_{12}$ + $C_{11}H_{22}$ isomer
66	211	n-undecane
67	212	C_5-alkyl benzene + $C_{12}H_{24}$ isomer
68	213	acetophenone
69	214	$C_{12}H_{26}$ isomer
70	215	$C_{12}H_{26}$ isomer
71	216	pentamethylheptane isomer
72	216	C_4-alkyl benzene
73	217	$C_{12}H_{24}$ isomer + silane compound
74	218	C_5-alkyl benzene
75	219	C_5-alkyl cyclohexane
76	220	$C_{12}H_{26}$ isomer
77	220.5	C_5-alkyl benzene
78	221	$C_{12}H_{26}$ isomer
79	222	C_5-alkyl benzene + methylindan
79A	223	dimethylundecane isomer
79B	223	1,2,3,4-tetrahydronaphthalene + C_5-alkyl benzene

(continued)

Table 45 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
80	224	$C_{13}H_{26}$ isomer
81	225	$C_{12}H_{24}$ isomer
82	226	n-dodecane
82A	227	dimethylindan
82B	227.5	C_5-alkyl benzene
83	228-229	naphthalene
85	232	C_6-alkyl benzene
85A	233	silane compound (BKG)
86	235	C_6-cyclohexane
90	240	n-tridecane
92	isothermal	β-methylnapthalene
93	isothermal	α-methylnaphthalene
96	isothermal	1-tetradecene
97	isothermal	n-tetradecane
99	isothermal	n-pentadecane

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[a] A 400 ft stainless steel SCOT capillary coated with OV-101 stationary phase was used for resolving pollutants. Capillary was programmed from 20-240°C @ 4°C/min. Carrier (He) gas was ~3.0 ml/min. See Table 29 (S5, duplicate) for sampling protocol.

Table 46. POLLUTANTS IDENTIFIED IN DAY AMBIENT AIR IN PASADENA, TX[a]

Chromatographic Peak No.a	Elution Temperature (°C)	Compound
1	34	n-propane
2	37	acetaldehyde
3	39	n-pentane
4	41	methylene chloride
5	43	acetone
6	46	3-methylpentane
7	48	C_6H_{14} isomer
8	50	n-hexane
9	51	chloroform
10	54	C_7H_{16} isomer
10A	56	1,1,1-trichloroethane
11	57	2-butanone
12	58	benzene
12A	58	carbon tetrachloride
13	59	cyclohexane
14	60	C_7H_{16} isomer
15	62	C_7H_{16} isomer
16	64	C_7H_{14} isomer
16A	65	trichloroethylene
17	66	n-heptane
18	70	C_7H_{14} isomer
19	72	C_7H_{14} isomer
20	77	toluene
21	78	2-methylheptane
22	80	3-methylheptane
23	82	C_8H_{16} isomer
24	84	n-octane
25	86	tetrachloroethylene
26	89	C_9H_{20} isomer
27	90	C_9H_{20} isomer
28	91	chlorobenzene

(continued)

Table 46 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
29	94	ethyl benzene
30	96	p-xylene
31	98	C_9H_{20} isomer
32	100	styrene
33	100	o-xylene
34	103	n-nonane
35	106	cumene
36	108	C_9H_{18} isomer
37	109	α-pinene
38	112	n-propylbenzene
39	113	m-ethyltoluene
40	114	1,3,5-trimethylbenzene
40A	115	benzaldehyde
41	116	o-ethyltoluene
42	119	1,2,4-trimethylbenzene
43	121	n-decane
43A	122	m-dichlorobenzene
44	124	1,2,3-trimethylbenzene
45	125	$C_{11}H_{24}$ isomer
46	126	C_9H_{10} isomer
47	127	$C_{10}H_{20}$ isomer
48	128	C_4-alkyl benzene
49	130	C_4-alkyl benzene
50	131	acetophenone
51	132	C_4-alkyl benzene
52	133	C_4-alkyl benzene
53	134	$C_{10}H_{12}$ isomer
54	136	C_4-alkyl benzene
55	137	n-undecane
56	139	C_4-alkyl benzene
57	140	C_4-alkyl benzene

(continued)

Table 46 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
58	141	C_4-alkyl benzene
59	142	C_5-alkyl benzene
60	143	C_5-alkyl benzene
61	143	$C_{10}H_{12}$ isomer
62	144	C_5-alkyl benzene
63	145	$C_{10}H_{12}$ isomer
64	146	C_5-alkyl benzene
65	147	C_5-alkyl benzene
66	148	C_5-alkyl benzene
67	150	naphthalene
68	151	$C_{11}H_{14}$ isomer
69	152	C_5-alkyl benzene
70	152	n-dodecane
71	155	$C_{13}H_{28}$ isomer
72	156	C_6-alkyl benzene
73	157	C_6-alkyl benzene
74	159	C_6-alkyl benzene
75	160	$C_{13}H_{28}$ isomer
76	162	$C_{11}H_{14}$ isomer
77	163	C_6-alkyl benzene
78	164	$C_{13}H_{28}$ isomer
79	166	β-methylnaphthalene
80	167	n-tridecane
81	169	$C_{13}H_{26}$ isomer
82	170	α-methylnaphthalene
83	171	$C_{14}H_{28}$ isomer
84	172	C_7-alkyl benzene
85	174	$C_{13}H_{26}$ isomer
86	175	$C_{14}H_{30}$ isomer
87	176	$C_{14}H_{30}$ isomer
88	177	$C_{14}H_{28}$ isomer

(continued)

Table 46 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
89	178	$C_{15}H_{32}$ isomer
90	179	$C_{14}H_{28}$ isomer
91	180	_n_-tetradecane

[a] A 42 m glass SCOT capillary coated with OV-101 was used. Capillary was programmed from 20-220°C @ 4°C/min. Carrier (He) was ~1.5 ml/min. See Table 29 (S5) for sampling protocol.

Table 47. POLLUTANTS IDENTIFIED IN NIGHT AMBIENT AIR IN TEXAS CITY, TX[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	71	CO_2
2	73	chlorodifluormethane
3	79	C_4H_8 isomer
4	87	isobutane
5	92	1,4-pentadiene
5A	93	n-pentane
5B	94	acetaldehyde
5C	95	methylene chloride
6	96	propanal and CS_2
7	97-105	acetone
10	109	chloroform
12	115	n-hexane
13	116	methyl cyclopentane
14	117	silane compound
15	121	C_7H_{16} isomer
15A	122	benzene
15B	122	cyclohexane and CCl_4 and methylcyclopropyl ketone
16	123	cyclohexene
17	124	2,4-dimethylpentane
18	125	2,3-dimethylpentane
19	126	3-methylhexane
21	129	1,cis-3-dimethylcyclopentane
21A	130	1,trans-2-dimethylcyclopentane
22	132	n-heptane
23	136-137	dimethyl-2-pentene isomer
24	138	C_8H_{16} isomer
25	139	C_8H_{18} isomer
26	141	C_7H_{14} isomer
27	143	1,trans-2,cis-3-trimethylcyclopentane
28	144	2,3-dimethylhexane

(continued)

Table 47 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
29	144-146	toluene
30	147	C_8H_{18} isomer
31	148	3-methylheptane
32	150	C_8H_{16} isomer
33	152	C_8H_{16} isomer
34	153	3-methyl-3-ethylpentane
34A	154	_n_-octane
35	155-156	hexamethylcyclotrisiloxane
38	161	C_8H_{16} isomer
39	162	C_9H_{18} isomer
40	165-166	ethyl benzene
41	167-168	_p_-xylene
42	169	C_9H_{20} isomer
42A	170	phenyl acetylene
43	172-173	styrene and 2-methyl-1-octene
44	173-175	_o_-xylene and _n_-nonane
46	180	isopropylbenzene
47	181	C_9H_{20} isomer
47A	181	propylcyclohexane
48	182	$C_{10}H_{16}$ isomer
49	184-185	_n_-propylbenzene
50	185	_m_-ethyltoluene
51	186	_p_-ethyltoluene
52	187	3-methyl-nonane
53	188-189	1,3,5-trimethylbenzene and $C_{10}H_{22}$ isomer
54	190	_o_-ethyltoluene
55	190-195	benzaldehyde
56	192-193	1,2,4-trimethylbenzene and _n_-decane
57	194	phenol
58	195	isobutylbenzene

(continued)

Table 47 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
59	196	dichlorobenzene isomer
60	197	t-butylbenzene
61	198	1,2,3-trimethylbenzene
62	199	$C_{11}H_{24}$ isomer
63	200	$C_{10}H_{20}$ isomer
64	201	β-methylstyrene
65	202	$C_{11}H_{22}$ isomer
66	202	sec-butylbenzene
67	203	_o_-cymene
68	204	$C_{11}H_{24}$ isomer
69	205	$C_{11}H_{24}$ isomer
70	206	C_4-alkyl benzene isomer
71	207	_m_-cymene
72	207	_p_-cymene
73	208	C_4-alkyl benzene isomer
74	209	_n_-undecane
75	210	acetophenone
76	211	C_5-alkyl benzene isomer
77	212-213	C_4-alkyl benzene isomer
78	213	$C_{12}H_{26}$ isomer
79	214	$C_{12}H_{26}$ isomer
80	215	C_4-alkyl benzene isomer
81	216	C_4-alkyl benzene isomer
82	217	C_5-alkyl benzene isomer
83	218	$C_{11}H_{22}$ isomer
83A	218	$C_{12}H_{26}$ isomer
84	219	methylindan isomer
85	220	C_5-alkyl benzene isomer
86	220	methylundecane isomer
87	221	dimethylstyrene isomer
88	222	$C_{12}H_{26}$ isomer

(continued)

Table 47 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
89	224	C_5-alkyl benzene isomer
90	224	$C_{12}H_{24}$ isomer
91	225-226	n-dodecane
92	227	dimethylindan isomer
93	228	naphthalene
94	228	$C_{13}H_{28}$ isomer
95	229	dimethylisopropylbenzene
96	231	C_6-alkyl benzene isomer
97	234	C_6H_{13}-cyclohexane isomer
98	235	1,2,4-trichlorobenzene
99	236	$C_{13}H_{28}$ isomer
100	237	silane compound
101	238	$C_{13}H_{28}$ isomer
102	239	C_6-alkyl benzene isomer and methyl-1,2,3,4-tetrahydronapthalene isomer
103	241	n-tridecane
104	242	$C_{13}H_{26}$ and C_5-alkyl benzene isomer
105	244	silane compound
106	246	methyl naphthalene (β)
107	249	methyl naphthalene (α)
108	251	C_7-alkyl cyclohexane
109	251	$C_{14}H_{30}$ isomer
110	252	$C_{14}H_{30}$ isomer
111	253	$C_{15}H_{32}$ isomer
112	255	1-tetradecene
113	256	n-tetradecane
114	257	biphenyl
117	261	ethyl naphthalene isomer
119	264	dimethylnaphthalene isomer
120	266	dimethylnaphthalene isomer
121	267	$C_{14}H_{28}$ isomer

(continued)

Table 47 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
122	268	C_8-alkyl cyclohexane isomer
124	273	n-pentadecane
132	291	n-hexadecane

[a] A 400 ft stainless steel SCOT coated with OV-101 was used for resolving the pollutants. Capillary was programmed from 20-240°C @ 4°C/min. Carrier (He) gas was ~3.0 ml/min. See Table 29 (S6) for sampling protocol.

Table 48. POLLUTANTS IDENTIFIED OR DETECTED IN AMBIENT AIR FROM TEXAS CITY, TX[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	78	carbon dioxide
1A	79	sulfur dioxide
2	82	propane
2A	83	1-butene
3	84	_n_-butane
4	85	2-butene
5	88	isopentane
6	93	_n_-pentane
7	96	acetone
8	104	methylene chloride
9	108	C_6H_{14} isomer
10	111	C_6H_{12} isomer
11	112	3-methylpentane
12	113	3-methylfuran
13	114	C_6H_{14} isomer
14	116	chloroform
15	118	C_6H_{12} isomer
16	119	C_7H_{16} isomer
17	120	methylcyclopentane
17A	121	ethyl acetate
17B	122	_n_-butanol
18	124	1,1,1-trichloroethane
19	126	C_7H_{16} isomer
19A	126	carbon tetrachloride
20,20A	130,131	C_7H_{16} isomer
21,21A	132	C_7H_{14} isomer
22	134	_n_-heptane
23	141	C_7H_{14} isomer
24,25	142	C_8H_{18} isomer

(continued)

Table 48 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
26	143	C_7H_{14} isomer
27,28	145,146	C_8H_{16} isomer
29	149	toluene
30	151	C_8H_{18} isomer
31-33	153,154	C_8H_{16} isomers
34	155	C_8H_{18} isomer
35	157	*n*-octane
36	158	C_8H_{16} isomer
37	159	unknown
38	159	tetrachloroethylene
39	161	C_8H_{16} isomer
40	162	C_9H_{20} isomer
41	164	C_9H_{18} isomer
42	165	C_8H_{16} isomer
43,44	166,167	C_9H_{18} isomer
45	168	chlorobenzene
46	169	C_9H_{18} isomer
47	170	C_9H_{20} isomer
48	171	ethylbenzene
49	172	*p*-xylene
50	173	*m*-xylene
51	173	phenyl acetylene
52,53	174,175	C_9H_{18} isomer
54	176	styrene
55	176	*o*-xylene
56	177	*n*-nonane
57	179	C_9H_{18} isomer
58,59	180,182	$C_{10}H_{22}$ isomers
60	182	isopropylbenzene
61	183	$C_{10}H_{22}$ isomer

(continued)

Table 48 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
62	184	C_9H_{18} isomer
63	185	β-pinene
64	186	$C_{10}H_{20}$ isomer
65	187	*n*-propylbenzene
66	189	*m*-ethyltoluene
67	190	*p*-ethyltoluene
68	191	$C_{10}H_{22}$ isomer
69	192	benzaldehyde
70	193	1,3,5-trimethylbenzene
71	194	$C_{10}H_{20}$ isomer
72	195	1,2,4-trimethylbenzene
72A	195	*n*-decane
73	197	$C_{11}H_{22}$ isomer
74	198	$C_{11}H_{24}$ isomer
74A	198	C_4-alkyl benzene
75	199	*m*-dichlorobenzene
76	199	C_4-alkyl benzene
77	201	1,2,3-trimethylbenzene
78	202	$C_{10}H_{20}$ isomer
79	203	$C_{11}H_{22}$ isomer
80	203	methyl styrene
81,82,83	204,205,206	C_4-alkyl benzenes
84	207	$C_{11}H_{24}$ isomer
85-89	208,209,210,211	C_4-alkyl benzenes
90	212	$C_{11}H_{24}$ isomer
90A	212	$C_{10}H_{12}$ isomer
91	213	C_5-alkyl benzene
92,93	214,215	C_4-alkyl benzene
93A	216	C_5-alkyl benzene
94-96	217,218	C_4-alkyl benzene

(continued)

Table 48 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
97-99	218,219	C_5-alkyl benzenes
100	221	$C_{10}H_{12}$ isomer
101-106	222,223,224,225,226	C_5-alkyl benzenes
107	227	C_6-alkyl benzene
108	228	n-dodecane
109	230	C_5-alkyl benzene
109A	230	tetrahydronaphthalene
110	230	C_5-alkyl benzene
111	230	naphthalene
112,113	230	C_5-alkyl benzenes
114	230	C_6-alkyl benzene
115	230	C_5-alkyl benzene
115A	230	C_6-alkyl benzene
116	230	C_6-alkyl benzene
117	230	C_5-alkyl benzene
118-120	230	C_6-alkyl benzenes
121-123	230	$C_{13}H_{28}$ isomers
124	230	$C_{14}H_{30}$ isomer

[a] Resolution was on a 400 ft OV-101 SCOT programmed from 20-230°C at 4°C/min, see Table 29 (S7) for sampling protocol.

Table 49. ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR IN PASADENA, TX[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	86	acetaldehyde
2	87-92	silane compound (BKG)
2A	92	propanal
2B	93-100	acetone
2C	98	3-methylpentane
3	101	2-methylfuran
3A	101	*n*-hexane
3B	102	methylpentane isomer
4	103	3-methylfuran and $CHCl_3$
5	106	methylcyclopentane and C_6H_{14} isomer
6	109	C_7H_{16} isomer
7	111	1,1,1-trichloroethane
7A	112	methyl ethyl ketone
7B	112	C_7H_{12} isomer
8	113	benzene
8A	113	CCl_4
9	114	cyclohexane
10	116	C_7H_{16} isomer
10A	117	2,3-dimethylpentane
10B	117	C_7H_{14} isomer
11	118	C_7H_{14} isomer
12	120	dimethylcyclopentane
13	121	trichloroethylene
14	123	*n*-heptane
14A	124	2,5-dimethylfuran
14B	125	2,4-dimethylfuran
14C	125	C_8H_{16} isomer
15	128	C_7H_{14} isomer
15A	129	C_8H_{16} isomer
	130	C_8H_{18} isomer

(continued)

Table 49 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
16	130	2,4-dimethylhexane
16A	131	1-methylcyclohexane
17	133	C_8H_{16} isomer
18	134	1,2,3-trimethylcyclohexane
19	136	2-methyl-3-ethylpentane
20	136-137	toluene
21	137-138	2-methylheptane
22	140	3-methylheptane
23	142	dimethylcyclohexane isomer
24	143	C_8H_{18} isomer
24A	144	dimethyl formamide and C_8H_{16} isomer
25	144-146	*n*-octane
26	146-148	tetrachloroethylene and hexamethyl cyclotrisiloxane (BKG)
26A	149	2-hexanone
26B	150	4-vinylcyclohexane
27	152	C_8H_{16} isomer
27A	153	C_9H_{20} isomer
27B	155	chlorobenzene
28	156-157	ethylbenzene
29	157-159	*p*-xylene
30	159	C_9H_{20} isomer
31	160	phenyl acetylene
32	162	C_9H_{18} isomer
33	162-163	*o*-xylene
34	163-165	*n*-nonane
35	168	C_9H_{18} isomer
36	169	isopropylbenzene
37	170	2,3-dimethyloctane
38	171	*n*-propylcyclohexane and $C_{10}H_{20}$ isomer

(continued)

Table 49 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
38A	172	$C_{10}H_{22}$ isomer
39	173	diisoamylene
40	174	n-propyl benzene
41	175	m-ethyl toluene and $C_{10}H_{22}$ isomer
42	176	p-ethyl tolene
43	177	1,3,5-trimethylbenzene
44	177	$C_{10}H_{22}$ isomer
44A	178	octamethylcyclotetrasiloxane (BKG)
45	178	$C_{11}H_{24}$ isomer
46	179	o-ethyltoluene
47	180	$C_{10}H_{20}$ isomer
48	181-183	1,2,4-trimethylbenzene and n-decane
49	183-190	benzaldehyde and phenol
50	185	isobutylbenzene
51	185-186	sec-butylbenzene and m-dichlorobenzene
52	186	$C_{11}H_{24}$ isomer and ter-butylbenzene
53	187	1,2,3-trimethylbenzene
54	188-189	$C_{10}H_{20}$ isomer
55	189	sec-butylcyclohexane
56	190	methyl styrene isomer
56A	190	o-dichlorobenzene and o-cymene
57	191	C_4-alkyl benzene isomer
58	191-192	C_4-alkyl benzene isomer
59	192	n-butyl benzene
60	193	methyl decane isomer
61	194	$C_{11}H_{24}$ isomer
62	194	C_4-alkyl benzene isomer
62A	195	$C_{10}H_{18}$ isomer

(continued)

Table 49 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
63	196	C_4-alkyl benzene isomer
64	196	C_4-alkyl benzene isomer
65	197	dimethyl styrene isomer and 5-undecene
66	198-199	n-undecane
66A	200-204	acetophenone
67	200	C_5-alkyl benzene isomer
67A	200	$C_{11}H_{22}$ isomer
67B	201	C_5-alkyl benzene isomer
68	201-202	$C_{12}H_{26}$ isomer
69	203	C_4-alkyl benzene isomer
70	203-204	$C_{11}H_{20}$ isomer
71	204	silane compound
72	205	C_5-alkyl benzene isomer
73	206	$C_{11}H_{24}$ isomer
74	206	C_5-alkylcyclohexane isomer
74A	206	ethylstyrene isomer
76	208	$C_{12}H_{24}$ isomer
76A	208	$C_{12}H_{26}$ isomer
77	209	C_5-alkyl benzene isomer
78	210	$C_{11}H_{24}$ isomer
79	210	$C_{12}H_{24}$ isomer
80	211	C_5-alkyl benzene isomer
81	212	$C_{12}H_{24}$ isomer
82	213	1-dodecene
83	213-215	n-dodecane
84	215-216	naphthalene
85	216	C_5-alkyl benzene isomer
86	219	C_6-alkyl cyclohexane isomer
88	220	$C_{11}H_{14}$ isomer
	221	$C_{12}H_{24}$ isomer

(continued)

Table 49 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
89	222	C_6-alkyl benzene isomer
90	223	$C_{13}H_{28}$ isomer
91	224	$C_{11}H_{14}$ isomer
92	224	$C_{13}H_{28}$ isomer
93	225	C_6-alkyl benzene isomer
94	227	$C_{11}H_{14}$ isomer and C_6-alkyl benzene isomer
95	228-229	n-tridecane
96	230	$C_{14}H_{28}$ isomer
97	231	$C_{14}H_{30}$ isomer
98	232	β-methyl naphthalene
99	233	C_7-alkyl benzene isomer
100	235	α-methyl naphthalene
103	238	benzothiazole
104	239	$C_{15}H_{32}$ isomer
107	240	n-tetradecane
108	isothermal	biphenyl
110		ethylnaphthalene isomers
111		dimethyl naphthalene isomer
112		dimethyl naphthalene isomer
116		n-pentadecane
122	↓	n-hexadecane

[a] See Table 29 (38) for sampling protocol.

Table 50. POLLUTANTS IDENTIFIED OR DETECTED IN AMBIENT AIR FROM MAY STREET, HOUSTON, TX[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	76	propene
2	79	cyclopropane
2A	79	chloromethane
3	80	2-methylpropane
3A	81	2-methylpropene
4	82	n-butane
5	83	trans-2-butene
6	84	cis-2-butene
7	87	ethyl chloride
8	91	isopentane
8A	91	trichlorofluoromethane
8B	91	propanal
9	92	acetone
10	96	methylene chloride
11	97	isopropanol
11A	98	C_6H_{12} isomer
12	104	C_6H_{12} isomer
13	107	3-methylpentane
14	108	4-methyl-1-pentene
15	109	C_6H_{14} isomer
16	111	n-hexane
17	113	chloroform
18	116	C_6H_{12} isomer
19	117	ethyl acetate
19A	118	C_5H_{10} isomer
19B	119	1,1,1-trichloroethane
20	123	C_7H_{16} isomer
21	124	carbon tetrachloride
22,22A,22B	126	C_7H_{16} isomers

(continued)

Table 50 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
22C,23	128,129	C_7H_{14} isomers
23A,23B	130,131	C_7H_{14} isomers
24	132	n-heptane
25	138	dimethylpentene
25A	139	C_8H_{18} isomer
25B	140	C_8H_{16} isomer
25C	140	C_8H_{18} isomer
26,27	142,144	C_7H_{14} isomers
28	145	C_7H_{16} isomer
29	146	toluene
30	149	C_8H_{18} isomer
31,32,33,34	151,152,153	C_8H_{16} isomer
35	153	C_8H_{18} isomer
36	154	n-octane
37	156	C_8H_{16} isomer
38	158	tetrachloroethylene
39,40,41	159,160	C_9H_{20} isomers
42	162	C_9H_{18} isomer
43	163	C_9H_{20} isomer
44,45,46	164,165,166	C_9H_{18} isomers
47	167	C_9H_{20} isomer
48	169	ethylbenzene
48A	170	p-xylene
48B	171	m-xylene
49,50	173	C_9H_{18} isomers
50A	173	bromoform (tent.)
51	174	C_9H_{18} isomer
52	176	o-xylene
52A	177	n-nonane
53	178	C_9H_{18} isomer
54	179	C_9H_{18} isomer

(continued)

Table 50 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
55	179	C_9H_{18} isomer
56	181	$C_{10}H_{22}$ isomer
57	181	isopropylbenzene
58,59	182,183	$C_{10}H_{22}$ isomers
60	184	C_9H_{18} isomer
61,62	184,185	$C_{10}H_{20}$ isomer
63	180	_n_-propylbenzene
63A	190	_m_-ethyltoluene
63B	191	_p_-ethyltoluene
63C,63D	192,193	$C_{11}H_{24}$ isomers
63E	193	1,3,5-trimethylbenzene
63F	193	benzaldehyde
64	194	$C_{10}H_{20}$ isomer
65	195	1,2,4-trimethylbenzene
66	197	$C_{10}H_{20}$ isomer
67	198	C_4-alkyl benzene
67A	198	_m_-dichlorobenzene
68	199	C_4-alkyl benzene
68A	199	unknown
69	200	1,2,3-trimethylbenzene
70	203	$C_{10}H_{20}$ isomer
71	204	C_9H_{10} isomer
72,72A,72B	206,207	C_4-alkyl benzenes
72C	207	$C_{12}H_{26}$ isomer
73,74,75,75A	208,210	C_4-alkyl benzenes
76,76A	211	C_4-alkyl benzenes
77,77A,78	213,214,215	C_5-alkyl benzenes
79	216	$C_{12}H_{24}$ isomer
80,81,82	217,218	C_4-alkyl benzenes
83,84	219,220	C_5-alkyl benzenes

(continued)

Table 50 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
85	221	$C_{10}H_{12}$ isomer
86-90	222,223,224,225,226	C_5-alkyl benzenes
91	227	C_6-alkyl benzenes
92	228	$C_{12}H_{26}$ isomer
93	229	C_5-alkyl benzene
94	230	$C_{13}H_{28}$ isomer
95	230	naphthalene
95A	230	C_5-alkyl benzene
95B	230	C_6-alkyl benzene
96	230	$C_{13}H_{26}$ isomer
97-100	230	C_6-alkyl benzenes
101	230	$C_{13}H_{26}$ isomer
102,103	230	C_6-alkyl benzenes
104	230	$C_{13}H_{28}$ isomer
105,106	230	C_6-alkyl benzenes
107	230	$C_{13}H_{28}$ isomer

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[a] Resolution was on a 400 ft OV-101 SCOT programmed from 20-230°C at 40°C/min, see Table 29 (S9) for sampling protocol.

Table 51. POLLUTANTS IDENTIFIED IN DAY AMBIENT AIR IN DOWNTOWN ST. LOUIS, MO[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	84	methylsilane
2	89	acetone
4	96	2-methylfuran and *n*-hexane
4A	97	3-methyl-2-pentene
5	98	3-methylfuran
5A	98	chloroform
6	100	vinyl isopropyl ether
7	102	C_7H_{16} isomer
8	104	C_6H_{14} isomer
9	106	1,1,1-trichloroethane
9A	107	methyl ethyl ketone
10	108	benzene and CCl_4
11	109	cyclohexane
12	110	2-methylhexane
13	111	C_7H_{16} isomer
13A	111	C_7H_{14} isomer
14	113	3-methylhexane
15	115	C_7H_{14} isomer
16	116	dimethylcyclopentane isomer
16A	117	trichloroethylene
17	119	*n*-heptane
17A	120	C_7H_{16} isomer
17B	121	C_7H_{12} isomer
17C	122	2,4-dimethylfuran
18	124	methylcyclohexane
19	126	C_8H_{16} isomer
19A	126	C_8H_{18} isomer
20	127	2,4-dimethylhexane
21	129	C_8H_{16} isomer
22	130	trimethylcyclopentane
22A	131	C_8H_{16} isomer

(continued)

Table 51 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
23	132	C_8H_{18} isomer
24	132-133	toluene
25	133-134	2-methylheptane
26	136	3-methylheptane
26A	137	dimethylcyclohexane isomer
27	138	C_8H_{16} isomer
27A	138	dimethylformamide
28	140	1-methyl-3-ethylcyclopentane
29	141-143	n-octane
29A	143	tetrachloroethylene
30	144	hexamethylcyclotrisiloxane
31	146	2-hexanone
32	148	C_9H_{20} isomer
32A	149	C_9H_{20} isomer
33	150	C_8H_{16} isomer
33A	151	C_9H_{18} isomer
34	152	chlorobenzene
35	153-154	ethylbenzene
36	154-156	p-xylene
37	157	C_9H_{20} isomer
37A	158	phenylacetylene
37B	159	styrene and C_9H_{18} isomer
38	160-161	o-xylene
39	161-163	n-nonane
39A	164	C_9H_{18} isomer
40	166	$C_{10}H_{22}$ isomer
41	168	isopropylbenzene
42	169	3-methylnonane
43	170	propylcyclohexane
44	171	$C_{10}H_{16}$ isomer
45	172-173	n-propylbenzene
46	173	m-ethyltoluene

(continued)

Table 51 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
47	174	p-ethyltoluene
48	175	1,3,5-trimethylbenzene
49	176	$C_{10}H_{22}$ isomer
50	177	octamethylcyclotetrasiloxane
51	178	o-ethyltoluene
52	179	1-methyl-4-isopropylcyclohexane
53	180-181	1,2,4-trimethylbenzene and n-decane
53A	181	benzaldehyde
53B	182	isobutylbenzene and $C_{10}H_{20}$ isomer
54	183-184	m-dichlorobenzene
55	184	methyldecane isomer
56	185	methyldecane isomer
57	186	1,2,3-trimethylbenzene and o-cymene
58	187	$C_{11}H_{24}$ isomer
59	188	sec-butylcyclohexane
60	188	o-methylstyrene
60A	189	o-dichlorobenzene and p-cymene
61	190	C_4-alkyl benzene isomer
62	190-191	m-diethylbenzene
63	191.5	n-butylbenzene
64	192	$C_{11}H_{24}$ isomer
65	192	$C_{11}H_{24}$ isomer
66	193	p-propyltoluene
67	194	$C_{10}H_{18}$ isomer
68	195	C_4-alkyl benzene isomer
69	195	C_4-alkyl benzene isomer
70	196	$C_{11}H_{22}$ isomer
71	197-198	n-undecane
72	199	C_5-alkyl benzene isomer and $C_{11}H_{22}$ isomer

(continued)

Table 51 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
73	200-201	C_5-alkyl benzene isomer
74	202	dimethylethylbenzene isomer
74A	202	$C_{12}H_{26}$ isomer
75	203	dimethylethylbenzene isomer
76	204	tetramethylbenzene and $C_{11}H_{20}$ isomer
77	205	C_5-alkyl benzene isomer
78	205	C_5-alkyl cyclohexane isomer
78A	205	C_5-alkyl benzene isomer
78B	206	dimethylstyrene isomer
79	206	C_5-alkyl benzene isomer
80	207	$C_{12}H_{26}$ isomer
81	208	C_4-alkyl benzene and C_5-alkyl benzene isomer
82	209	$C_{12}H_{26}$ isomer
83	210	C_5-alkyl benzene isomer
84	211	C_5-alkyl benzene isomer and $C_{13}H_{28}$ isomer
85	212	1-dodecene
86	213	n-dodecane
86A	214	naphthalene
87	216	$C_{13}H_{28}$ isomer
88	217	$C_{13}H_{28}$ isomer
89	218	C_6-alkyl benzene isomer
89A	219	1,3,5-trichlorobenzene
90	220	$C_{13}H_{26}$ isomer
91	221	$C_{12}H_{24}$ isomer
92	222	C_6-alkyl benzene isomer
93	223	$C_{13}H_{28}$ isomer
94	224	$C_{13}H_{28}$ isomer

(continued)

Table 51 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
95	225	$C_{13}H_{28}$ isomer
96	228	_n_-tridecane
103	240	_n_-tetradecane

[a] A 400 ft OV-101 stainless steel SCOT was programmed from 20-240°C @ 4°C/min. Air samples were taken on balcony of 32nd floor apartment. See Table 30 (S3) for sampling protocol.

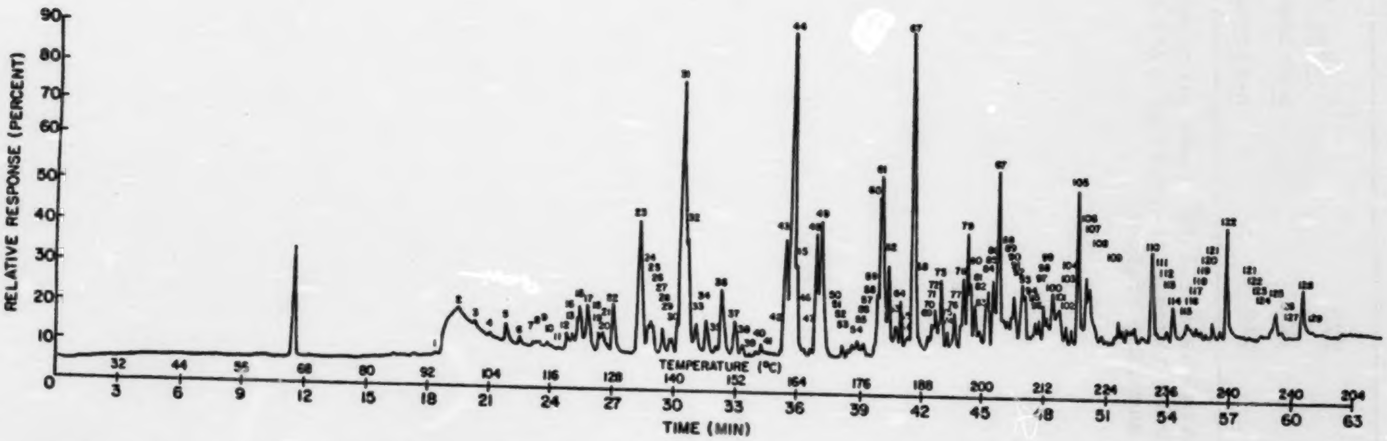

Figure 33. Profile of ambient air pollutants from Arvado, CO using high resolution gas chromatography/mass spectrometry/computer. A 400 ft S.S. SCOT coated with OV-101 stationary phase was used; temperature programmed from 20-240°C @ 4°C/ min. See Table 52 for listing.

Table 52. POLLUTANTS IDENTIFIED IN AMBIENT AIR FROM ARVADO, MO[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
0	62	carbon dioxide
1	69	sulfur dioxide
2	71	2-butene
3	82	C_5H_{12}
4	86	acetaldehyde
5	88	furan
6	92	propionaldehyde
7	96	C_6H_{14}
8	98	acetone
9	101	C_6H_{14}
10	104	*n*-hexane
11	106	2-methylfuran
12	107	C_6H_{12}
13	110	C_6H_{12}
14	114	1,1,1-trichloroethane
15	116	benzene
16	117	C_6H_{12}
17	118	C_7H_{12}
18	120	C_7H_{16}
19	122	C_7H_{14}
20	123	C_7H_{14}
21	124	trichloroethylene
22	125	C_7H_{16}
23	128	2,4-dimethylfuran
24	130	C_7H_{14}
25	132	C_8H_{18}
26	134	C_8H_{18}
27	135	C_8H_{16}
28	136	C_8H_{16}
29	137	toluene

(continued)

Table 52 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
30	138	C_8H_{18}
31	140	C_8H_{18}
32	142	C_8H_{16}
33	142	C_8H_{16}
34	143	C_8H_{16}
35	144	C_8H_{16}
36	145	C_8H_{18}
37	146	hexamethylcyclotrisiloxane
38	147	tetrachloroethylene
39	149	4-methyl-pentan-2-one
40	150	C_9H_{20}
41	151	C_9H_{20}
42	152	C_8H_{16}
43	153	C_9H_{20}
44	153	C_8H_{16}
45	154	C_9H_{18}
46	155	C_9H_{18}
47	155	chlorobenzene
48	156	C_9H_{18} (tent.)
49	156	ethylbenzene
50	157	C_9H_{20}
51	158	*p*-xylene
52	159	*m*-xylene
53	160	phenylacetylene
54	161	$C_{10}H_{22}$ (tent.)
55	162	styrene
55A	162	C_9H_{18}
56	163	*o*-xylene
57	164	C_9H_{20}
58	167	C_9H_{18}
59	168	$C_{10}H_{22}$

(continued)

Table 52 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
60	169	$C_{10}H_{22}$
61	169	$C_{10}H_{22}$
62	170	isopropylbenzene
62A	170	$C_{10}H_{22}$
63	170	$C_{10}H_{22}$
64	171	$C_{10}H_{22}$
65	171	C_9H_{18}
65A	171	$C_{10}H_{20}$
66	172	$C_{10}H_{22}$
66A	172	$C_{10}H_{20}$
66B	172	unknown
67	173	$C_{10}H_{20}$
68	174	$C_{10}H_{20}$
69	174	_n_-propylbenzene
70	175	_m_-ethyltoluene
71	175	_p_-ethyltoluene
72	176	1,3,5-trimethylbenzene
73	177	$C_{10}H_{22}$
74	177	unknown
75	178	$C_{10}H_{22}$ (tent.)
76	179	_o_-ethyltoluene
77	180	$C_{10}H_{20}$
78	181	1,2,4-trimethylbenzene
78A	181	$C_{10}H_{22}$
79	183	benzaldehyde
80	184	sec-butylbenzene
81	185	_m_-dichlorobenzene
82	186	_o_-cymene
82A	186	$C_{11}H_{24}$
83	187	1,2,3-trimethylbenzene
84	188	$C_{11}H_{24}$

(continued)

Table 52 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
85	189	$C_{10}H_{20}$
86	191	β-methylstyrene
87	193	$C_{11}H_{22}$
88	194	C_4-alkyl benzene
89	195	C_4-alkyl benzene
90	196	C_4-alkyl benzene
91	197	C_4-alkyl benzene
91A	197	$C_{11}H_{24}$
92	198	$C_{11}H_{24}$
93	200	C_4-alkyl benzene
93A	200	$C_{12}H_{26}$
94	201	$C_{11}H_{24}$
95	204	C_4-alkyl benzene
96	207	C_4-alkyl benzene
96A	207	$C_{12}H_{26}$
97	209	C_4-alkyl benzene
98	210	C_4-alkyl benzene
99	211	C_4-alkyl benzene
100	213	$C_{11}H_{22}$
101	214	$C_{11}H_{24}$
102	215	$C_{11}H_{24}$
103	216	$C_{11}H_{24}$
104	218	C_5-alkyl benzene
104A	218	$C_{11}H_{22}$
105	219	C_4-alkyl benzene
106	221	C_5-alkyl benzene
106A	221	$C_{12}H_{26}$
107	223	C_4-alkyl benzene
108	224	$C_{12}H_{26}$
109	226	C_4-alkyl benzene
110	227	unknown Si cpd. m/e 267, 281, 341

(continued)

Table 52 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
111	228	C_5-alkyl benzene
112	229	$C_{11}H_{22}$
113	230	C_5-alkyl benzene
114	231	C_4H_7-alkyl benzene
115	232	$C_{12}H_{26}$
116	233	C_5-alkyl benzene
117	237	C_4H_7-alkyl benzene
117A	237	$C_{12}H_{26}$
118	238	C_5-alkyl benzene
119	239	$C_{12}H_{22}$
120	240	$C_{12}H_{26}$
121	isothermal	C_5-alkyl benzene
122		$C_{12}H_{24}$
123		$C_{12}H_{26}$
124		C_5H_9-alkyl benzene
125		C_5-alkyl benzene
126		naphthalene
127		$C_{13}H_{28}$
128		C_5-alkyl benzene
129		$C_{13}H_{28}$
130		$C_{13}H_{28}$
131		C_6-alkyl benzene
132		C_6-alkyl benzene
132A		$C_{13}H_{26}$
133		C_6-alkyl benzene
134		$C_{13}H_{26}$
135		$C_{13}H_{28}$
136		$C_{13}H_{28}$
136A		C_6-alkyl benzene
137		$C_{13}H_{28}$
138		$C_{13}H_{26}$

(continued)

Table 52 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
139	isothermal	$C_{13}H_{28}$
140		$C_{14}H_{30}$
141		$C_{13}H_{28}$
142		$C_{14}H_{28}$
143		unknown, m/e 73
144		$C_{14}H_{30}$
145		$C_{14}H_{20}$
146		unknown
147		unknown
148		$C_{14}H_{30}$
149		$C_{15}H_{32}$ (tent.)
150		$C_{14}H_{30}$

[a] See Table 30 (S4) for sampling protocol.

Table 53. POLLUTANTS IDENTIFIED IN AMBIENT AIR FROM ST. ANN, MO[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
6	83	acetaldehyde
7	84	dichloromethane
8	86	carbon disulfide
9	87	propionaldehyde
10	89	acetone
11	92	hexane isomer
12	95	hexane isomer
13	98	hexane isomer
14	101	chloroform
15	104	hexene isomer
16	105	heptane isomer
17	107	heptane isomer
18	109	1,1,1-trichloroethane
19	111	benzene
20	112	cyclohexane
21	113	heptane isomer
22	113	heptane isomer
23	114	heptene isomer
24	115	heptane isomer
25	116	heptane isomer
26	117	heptene isomer
27	118	heptene isomer
28	120	trichloroethylene
29	121	heptane isomer
30	126	heptene isomer
31	128	octane isomer
32	128	octane isomer
33	130	octene isomer
34	132	heptene isomer
35	132	heptene isomer
36	133	octane isomer

(continued)

Table 53 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
37	134	toluene
38	135	octane isomer
39	137	octane isomer
40	139	nonane isomer
41	141	nonene isomer
42	142	octane isomer
43	144	tetrachloroethylene
44	145	unknown
45	146	unknown
46	148	unknown
47	149	nonane isomer
48	150	nonane isomer
49	151	octene isomer
50	153	nonene isomer
51	153	nonene isomer
52	154	chlorobenzene
53	154	ethylbenzene
54	155	p-xylene
55	157	m-xylene
56	158	phenyl acetylene
57	158	decane isomer
58	160	nonene isomer
59	161	o-xylene
60	162	n-nonane
61	165	nonene isomer
62	166	decane isomer
63	167	decane isomer
64	168	isopropylbenzene
65	168	decane isomer
66	169	decane isomer
67	169	nonane isomer
68	170	cyclofenchene (tent.)

(continued)

Table 53 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
69	171	decene isomer
70	172	n-propylbenzene
71	173	m-ethyltoluene
72	174	p-ethyltoluene
73	175	1,3,5-trimethylbenzene
74	175	decane isomer
75	177	unknown
76	178	o-ethyltoluene
77	179	decene isomer
78	180	1,2,4-trimethylbenzene
79	180	n-decane
80	181	benzaldehyde
81	183	C_4-alkyl benzene
82	184	m-dichlorobenzene
83	184	C_4-alkyl benzene
84	186	1,2,3-trimethylbenzene
85	187	undecane isomer
86	188	undecane isomer
87	188	o-methylstyrene (tent.)
88	189	undecene isomer
89	190	C_4-alkyl benzene
90	190	C_4-alkyl benzene
91	190	C_4-alkyl benzene
92	191	C_4-alkyl benzene
93	191	undecane isomer
94	192	dodecane isomer
95	193	C_4-alkyl benzene
96	194	dodecane isomer
97	195	C_4-alkyl benzene
98	196	C_4-alkyl benzene
99	197	n-undecane
99A	197	methyl indan isomer

(continued)

Table 53 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
100	198	C_5-alkyl benzene
101	199	undecene isomer
102	200	C_5-alkyl benzene
102A	200	dodecane isomer
103	201	C_4-alkyl benzene
104	202	tridecane isomer
105	203	unknown
106	204	dodecane isomer
107	204	C_5-alkyl benzene
108	205	undecene isomer
108A	205	C_5-alkyl benzene
109	206	methylindan isomer
110	207	C_5-alkyl benzene
111	207	dodecene isomer
112	207	C_5-alkyl benzene
113	208	dodecane isomer
114	209	C_5-alkyl benzene
115	210	C_5-alkyl benzene
116	210	C_5-alkyl benzene
117	211	dodecane isomer
118	212	n-dodecane
119	214	naphthalene
120	215	tridecane isomer
121	216	C_5-alkyl benzene
122	217	C_6-alkyl benzene
123	218	tridecane isomer
123A	218	tridecane isomer
124	219	C_6-alkyl benzene
125	220	unknown
126	221	dodecene isomer
127	222	C_6-alkyl benzene
128	222	tridecane isomer

(continued)

Table 53 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
129	223	tridecene isomer
129A	223	C_6-alkyl benzene
130	223	tridecane isomer
131	224	tridecane isomer
132	225	tridecene isomer
133	226	unknown
134	227	tridecane isomer
135	229	tridecene isomer
136	230	tetradecane isomer
137	231	β-methylnaphthalene
138	232	tetradecene isomer
139	234	α-methylnaphthalene
140	235	tetradecane isomer
141	236	tetradecane isomer
142	236	tetradecane isomer
143	237	pentadecane isomer
144	238	pentadecane isomer
145	240	tetradecene isomer
146	240	*n*-tetradecane
147	240	tetradecene isomer
148	240	tetradecene isomer
149	240	tetradecene isomer
150	240	hexadecane isomer
151	240	pentadecane isomer

[a] See Table 31 (S5) for sampling protocol.

Table 54. ORGANIC VAPORS IDENTIFIED IN DAY AMBIENT AIR AT THE ENTRANCE OF THE EISENHOWER TUNNEL IN COLORADO[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	100.5	2-methylfuran
2	103	_n_-hexane
2A	104	chloroform
4	107.5	methylcyclopentane
5A	111	1,1,1-trichloroethane
5B	112	$C_5H_{10}O$ isomer
6	113	benzene + carbon tetrachloride
7	114	cyclohexane
8	115	2-methylhexane
9	116	2,3-dimethylpentane
9A	116	1,1-dimethylcyclopentane
10	117	3-methylhexane
11	119.5	1,cis-3-dimethylcyclopentane
12	121	1,trans-2-dimethylcyclopentane
13	122	_n_-heptane
14	128	4,4-dimethyl-2-pentene
15	130	C_8H_{18} isomer
16	131	2,4-dimethylhexane
18	134	1,trans-2,cis-3-trimethylcyclopentane
20	136	2,3-dimethylhexane
21	137	toluene
22	137.5-9	C_8H_{18} isomer
23	140	3-methylheptane
23A	140	dimethylnitrosamine (tent.)
24	141	2,3,4-trimethyl-2-pentene
25A	143	dimethyl formamide + C_8H_{18} isomer
25B	143.5	1-methyl-3-ethylcyclopentane
26	144-6	_n_-octane
27	147	hexamethylcyclotrisiloxane (BKG)

(continued)

Table 54 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
28	149.5	tetrachloroethylene
28A	150	C_9H_{20} isomer
29	151	C_9H_{20} isomer
30	152	2,6-dimethylheptane
31	153	_n_-propylcyclopentane
32	154	C_9H_{18} isomer + C_9H_{20} isomer
33	155	C_9H_{18} isomer
33A	155.5	1-nonene
33B	156	2,3-dimethylheptane
33C	156.5	4-methyloctane
34	157	ethylbenzene
35	158	_p_-xylene
36	159	3-methyloctane
37	160	_o_-xylene
37A	161	phenyl acetylene
38	163.5	C_9H_{18} isomer
39	164-8	_n_-nonane
40	168.5	1-methyl-2-ethylcyclohexane
41	169	$C_{10}H_{22}$ isomer
42	170	2-methylnonane
43	171	C_3-alkyl benzene
44	171-2	3-methylnonane
45	173	propylcyclohexane + $C_{10}H_{22}$ isomer
46	174	$C_{10}H_{22}$ isomer
47	174.5	$C_{10}H_{20}$ isomer
48	175.5	$C_{10}H_{22}$ isomer
49	176.5	4-methylnonane
50	177	_p_-ethyltoluene
51	178	$C_{10}H_{20}$ isomer
52	178-9	$C_{10}H_{22}$ isomer
53	180	diethylcyclohexane isomer

(continued)

Table 54 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
55	181	*o*-ethyltoluene
56	182	1-methyl-trans-4-isopropylcyclohexane
57	183-4	*n*-decane + 1,2,4-trimethylbenzene
58	184.5	$C_{10}H_{20}$ isomer
59	185	benzaldehyde
60	186	5-methyldecane
60A	186	2-phenylpropionaldehyde (tent.) + C_4-alkyl benzene
61	187	methyldecane isomer
62	187-8	methyldecane isomer
63	189	1,2,3-trimethylbenzene
64	190	*t*-butylbenzene
65	191	$C_{11}H_{24}$ isomer
66	191	*n*-butylcyclohexane
67	192	$C_{11}H_{22}$ isomer
68	192.5	$C_{11}H_{22}$ isomer
69	193	C_4-alkyl benzene
70	193.5	*m*-diethylbenzene
71	194	*n*-undecane
72	195-6	*p*-propyltoluene
75	198	C_4-alkyl benzene
76	199	C_4-alkyl benzene + $C_{11}H_{24}$ isomer
77	199.5	C_4-alkyl benzene + $C_{11}H_{22}$ isomer
78	200	$C_{11}H_{22}$ + $C_{11}H_{24}$ isomer
79	202	C_5-alkyl benzene
80	202	$C_{11}H_{22}$ isomer
81	203	$C_{12}H_{26}$ isomer
82	204.5	acetophenone
83	205	$C_{12}H_{26}$ isomer

(continued)

Table 54 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
84	206	biphenylene (tent.)
84A	207	$C_{12}H_{24}$ isomer
85	208	C_5-alkyl benzene
86	208-9	$C_{12}H_{26}$ isomer
87	209	$C_{12}H_{24}$ + $C_{12}H_{26}$ isomers
88	210	C_5-alkyl benzene
89	210.5	$C_{12}H_{24}$ isomer
90	211	$C_{12}H_{26}$ isomer
91	212-3	2,3-dihydro-2-methylbenzofuran (tent.) + 2-phenyl-2-methylbutane
92	214	cyclodecane (tent.)
93	215	C_5-alkyl benzene
94	216	n-dodecane + decamethyltetrasiloxane (BKG)
96	218	1-methyl-3-t-butylbenzene
97	219	naphthalene + 1,3,5-trichlorobenzene
100	224	$C_{13}H_{26}$ isomer
105	231	n-tridecane
109	240	7-methyltridecane
111	240	n-tetradecane
112	240	n-pentadecane
113	240	n-hexadecane

[a] See Table 31 (S1) for sampling protocol.

Table 55. ORGANIC VAPORS IDENTIFIED IN DAY AMBIENT AIR IN DENVER, CO[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	87	methylene chloride
2	91	acetaldehyde
3	91	dimethylether
3A	92	diethylether
4	93	acetone
4A	95	C_6H_{14} isomer
4B	97	3-methylpentane
4C	98	1-hexene
5	100	n-hexane
5A	101	methyl furan
5B	101	C_6H_{12} isomer
6	102	$CHCl_3$
7	105	C_7H_{16} isomer
7A	105	C_6H_{12} isomer
8	106	C_7H_{16} isomer
9	107	C_7H_{16} isomer
9A	109	n-butanal
9B	110	1,1,1-trichloroethane
10	111	benzene
11	111	CCl_4
12	112	cyclohexane
13	113	C_7H_{16} isomer
13A	113	2,3-dimethylpentane
14	114	C_7H_{14} isomer
15	115	3-methylhexane
16	117	C_7H_{16} isomer
17	118	1,trans-2-dimethylcyclopentane
18	119	C_8H_{16} isomer
19	120	n-heptane
19A	123	C_7H_{12} isomer
20	124-125	methyl cyclohexane
21	126	C_8H_{18} isomer

(continued)

Table 55 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
22	127	C_8H_{18} isomer
23	127	C_7H_{14} isomer
24	129	trimethylcyclopentane isomer
25	130	trans-4-octene
26	131	trimethylpentane isomer
27	132	2,3-dimethylhexane
28	132-4	toluene
29	133-5	C_8H_{18} isomer
30	136	3-methylheptane
31	137	dimethylcyclohexane isomer
32	138	trimethylpentane isomer
33	139	1-octene
34	140-2	n-octane
35	143	tetrachloroethylene and trimethylcyclotrisiloxane
36	145	2-hexanone and C_9H_{20} isomer
37	146	C_9H_{20} isomer
38	147	Dimethylcyclohexene isomer
38A	147	2,6-dimethylheptane
39	148	C_8H_{16} isomer
40	148	C_8H_{16} isomer
41	149	C_9H_{18} isomer
42	150	1-nonene
43	152	C_9H_{20} isomer
44	152-3	ethyl benzene
45	153-4	p-xylene
46	155	phenyl acetylene and C_9H_{18} isomer
47	157	2,2,5-trimethylhexane
48	158	C_9H_{18} isomer
49	158-9	o-xylene
50	156-61	n-nonane

(continued)

Table 55 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
51	163	methylethylcyclohexane isomer
52	164	$C_{10}H_{22}$ isomer
53	165	2,5-dimethyloctane
54	165	isopropylbenzene and C_9H_{16} isomer
55	166	$C_{10}H_{22}$ isomer
56	167	C_3-alkyl cyclohexane isomer
57	168	α-pinene
57A	168	4-propylheptane
58	169	$C_{10}H_{20}$ isomer
58A	169	$C_{10}H_{22}$ isomer
59	170	n-propylbenzene
59A	171	$C_{10}H_{22}$ isomer
60	171-2	_m_-ethyltoluene
61	173	p-ethyltoluene and $C_{10}H_{22}$ isomer
62	174	$C_{10}H_{22}$ isomer
62A	174	$C_{11}H_{24}$ isomer
63	175	_o_-ethyltoluene
63A	176	1-decene
64	176	1-methyl-4-isopropylcyclohexane
65	177	1,2,4-trimethylbenzene and n-decane
66	178	benzaldehyde
66A	179	isobutylbenzene
67	181	sec-butylbenzene
68	181	_m_-dichlorobenzene
69	182	$C_{11}H_{24}$ isomer
70	182	_o_-cymene
71	183	1,2,3-trimethylbenzene
72	184	C_4-alkylcyclohexane isomer
73	185	β-methylstyrene

(continued)

Table 55 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
74	185	$C_{11}H_{22}$ isomer and m-diethylbenzene
75	187	p-propyltoluene
76	188	o-diethylbenzene
77	188	dimethylnonane isomer
78	189	2-methyldecane
79	189	$C_{11}H_{24}$ isomer
80	190	o-propyltoluene and $C_{10}H_{18}$ isomer
81	192	dimethylethylbenzene isomer
82	193	$C_{10}H_{12}$ isomer and 1-undecene
83	194	n-undecane
84	196	C_5-alkylbenzene and $C_{11}H_{22}$ isomer
84A	196	$C_{12}H_{26}$ isomer
85	197	C_4-alkylbenzene and C_5-alkylbenzene isomer
85A	198	acetophenone
86	198	C_4-alkylbenzene isomer
87	199	$C_{12}H_{26}$ isomer
	199	C_4-alkylbenzene isomer
88	200	$C_{12}H_{24}$ isomer
89	200	silane compound
90	201	C_5-alkylcyclohexane isomer
90A	201	C_5-alkyl benzene and $C_{12}H_{24}$ isomer
91	202	$C_{10}H_{22}$ isomer and $C_{12}H_{20}$ isomer
92	203	C_5-alkylbenzene isomer and $C_{10}H_{12}$ isomer
93	204	C_5-alkyl benzene isomer
94	205	$C_{12}H_{26}$ isomer

(continued)

Table 55 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
95	206	C_5-alkyl benzene isomer
95A	207	C_1[illegible]H_{24} isomer
96	208	1-dodecene
97	209	n-dodecane
97A	210	naphthalene
98	212	$C_{13}H_{28}$ isomer
99	213	$C_{13}H_{28}$ isomer
100	214	C_6-alkyl benzene isomer
102	216	$C_{13}H_{26}$ isomer
103	217	C_6-alkyl cyclohexane isomer
105	219	$C_{13}H_{28}$ isomer
106	220	$C_{13}H_{28}$ isomer
107	221	$C_{14}H_{30}$ isomer
108	222	silane compound
109	224	n-tridecane
111	227	$C_{14}H_{28}$ isomer
112	232	methyl naphtalene isomer
115	235	silane compound
117	237	n-tetradecane

[a] See Table 31 (S7) for sampling protocol.

Table 56. POLLUTANTS IDENTIFIED IN AMBIENT AIR IN PATERSON, NJ[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	72	$N_2 + O_2$
2	74	CO_2
2A	76	ethylene oxide
3	80	CF_2Cl_2
3A	84	propane
3B	86	isobutane
3C	90	1-butene
4	91	*n*-butane
4A	92	2-butene
4B	93	cyclobutane
5	95	acetaldehyde
6	100	silane compound (BKG)
7	103	isopentane
7A	104	CCl_3F
8	105	1-pentene
8A	106	furan
8B	107	trans-2-pentene
9	108	*n*-pentane
10	109	cis-2-pentene
11	112	CH_2Cl_2
11A	113	propanal
12	123	2-methylpentane
13	126	3-methylpentane
14	128	hexafluorobenzene (eS)
15	129	*n*-hexane
16	131	$CHCl_3$
17	134	perfluorotoluene (eS)
17A	135	C_6H_{14} isomer
18	137	methyl cyclopentane
18A	138	1,2-dichloroethane
19	139	1,1,1-trichloroethane

(continued)

Table 56 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
20	143	benzene
20A	143	CCl_4
20B	144	2-methylhexane
21	145	C_7H_{16} isomer
22	147	3-methylhexane
22A	148	C_7H_{14} isomer
23	151	dibromomethane
24	152	trichloroethylene
24A	153	_n_-heptane
25	160	methylcyclohexane
26	164	C_8H_{18} isomer
27	167	toluene
28	168	2,4-dimethylhexane
29	171	dimethylcyclohexane
30	173	_n_-octane
31	175	hexamethylcyclotrisiloxane (BKG)
32	177	tetrachloroethylene
33	181	C_9H_{18} isomer
34	184	chlorobenzene
34A	185	C_9H_{18} isomer
35	187	ethylbenzene
36	189	_p_-xylene
36A	191	_m_-xylene
36B	192	styrene
37	193-194	_o_-xylene and _n_-nonane
37A	195	methyl ethyl cyclohexane isomer
37B	193	C_9H_{18} isomer
38	199	isopropylbenzene
39	201	methylnonane isomer
39A	202	C_9H_{18} isomer
40	203	$C_{10}H_{16}$ isomer

(continued)

Table 56 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
41	204	n-propylbenzene
42	204-207	m-ethyltoluene
43	207-208	p-ethyltoluene
44	210	o-ethyltoluene
44A	210	menthene or $C_{10}H_{18}$ isomer
44B	211	methane or $C_{10}H_{20}$ isomer
45	211-212	1,2,4-trimethylbenzene
46	213	$C_{10}H_{20}$ isomer
47	216	n-decane
47A	217	o-cymene
48	218	1,2,3-trimethylbenzene
49	220	$C_{10}H_{20}$ isomer
50	221	C_4-alkyl benzene isomer
50A	222	$C_{11}H_{24}$ isomer
51	223	m-diethylbenzene
52	225	acetophenone and $C_{11}H_{24}$ isomer
53	228	C_4-alkyl benzene isomer
53A	228	$C_{10}H_{18}$ isomer
54	229	n-undecane

[a] See Table 35 (S1) for sampling protocol.

Table 57. POLLUTANTS IDENTIFIED IN AMBIENT AIR IN CLIFTON, NJ[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	80	dichlorodifluoromethane
1A	84	CH_3Cl
2	85	propene
2A	86	propane
2B	87	vinyl chloride
3	88	1-butene
4	90	n-butane
4A	91	2-butene
5	92-94	acetaldehyde
5A	94	cyclobutane
5B	94-100	methyl silane (BKG)
6	101-104	isopentane
7	104	CCl_3F
7A	105	1-pentene
7B	105	furan
7C	106	2-methyl-1-butene
8	106	C_5H_{10} isomer
9	107	n-pentane
9A	108	cis-2-pentene
10	110-117	acetone
10A	111	CH_2Cl_2
10B	118	2,2-dimethylbutane
11	122	2-methylpentane
12	126	3-methylpentane
13	128	hexafluorobenzene (S)
13A	128	2-methylfuran
14	129	n-hexane
14A	130	C_6H_{12} isomer
15	131	$CHCl_3$
16	132	C_5H_8O isomer
17	133-134	perfluorotoluene (S)

(continued)

Table 57 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
18	136	methyl ethyl ketone
19	137-140	1,2-dichloroethane
19A	141	1,1,1-trichloroethane
20	143	benzene
20A	143.5	CCl_4
21	144-145	2-methylhexane
22	146-147	3-methylhexane
23	149	C_7H_{14} isomer
24	150	trichloroethylene
25	151-153	_n_-heptane
26	157	C_7H_{16} isomer
27	159	methylcyclohexane
28	165	C_8H_{16} isomer
29	166-169	toluene
29A	168	C_8H_{18} isomer
30	171	C_8H_{16} isomer
30A	172	dimethylcyclohexane isomer
31	173-174	_n_-octane
32	175	hexamethylcyclotrisiloxane (BKG)
33	177	tetrachloroethylene
34	182	C_9H_{20} isomer
34A	183	methylethylcyclopentane isomer
35	184	chlorobenzene
36	187	ethylbenzene
37	189	_p_-xylene
38	191	1-nonene
39	193	styrene
40	193-195	_o_-xylene and _n_-nonane
40A	197	C_9H_{18} isomer
41	199	isopropylbenzene
43	204	$C_{10}H_{16}$ isomer

(continued)

Table 57 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
43A	205	n-propylbenzene
44A	206	benzaldehyde
44	207	m-ethyltoluene
45	208-209	octamethylcyclotetrasiloxane (BKG)
46	211	o-ethyltoluene
47	213	n-decane and 1,2,4-trimethylbenzene
48	217	m-dichlorobenzene
48A	218	C_4-alkyl benzene isomer
48B	219	1,2,3-trimethylbenzene
49	222	C_4-alkyl benzene isomer
50	224	C_4-alkyl benzene isomer
51	226	acetophenone
51A	227	C_4-alkyl benzene isomer
52	229	n-undecane
53	230	C_5-alkyl benzene isomer
54	237	silane compound (BKG)
55	240	n-dodecane

[a] See Table 35 (S2) for sampling protocol.

Table 58. ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR IN PASSAIC, NJ[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
2	75	CO_2
2A	76	ethylene oxide
2B	77	SO_2
2C	78	propene
3	80-82	CF_2Cl_2
3A	83	n-propane
3B	85	$CHCl_3$
3C	86	isobutane
4	88-89	vinyl chloride
4A	90	1-butene
5	91	n-butane
5A	92	2-butene (isomer)
6	94-96	acetaldehyde
6A	97	chloroethane
6B	99	C_5H_{12} (isomer)
6C	101	methyl ethyl ether
6C	102	methyl silane (BKG)
7	104	isopentane
8	105	trichlorofluormethane
8A	106	1-pentene
8B	107	furan and C_5H_{10} (isomer)
9	108-109	n-pentane
9A	110	methylcyclobutane
9B	111	propanal
10	113	C_5H_{10} (isomer)
10A	114-116	CH_2Cl_2 (isomer)
11	117-122	acetone
11A	122	isopropanol
12	123-124	2-methylpentene
13	126	2-methylfuran

(continued)

Table 58 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
13A	127	3-methylpentane
13B	127	C_6H_{12} (isomer)
14	128-129	hexafluorobenzene (S)
14A	129	C_6H_{12} (isomer)
15	129-131	n-hexane
15A	131	C_6H_{12} (isomer)
16	131-133	$CHCl_3$
17	134-136	perfluorotoluene (S)
18	137	2,4-dimethylpentane
18A	138	C_7H_{14} (isomer)
19	140-141	1,1,1-trichloroethane
19A	142	methyl ethyl ketone
20	144-145	benzene
20A	145	CCl_4
21	146	2-methylhexane
22	146-149	cyclohexane and dimethyl pentane (isomer)
22A	149	C_7H_{14} (isomer)
23	150-154	C_7H_{14} (isomer) and trichloroethylene and n-heptane
23A	156	C_8H_{16} (isomer)
24	160-162	C_8H_{16} (isomer)
24A	162	2,4-dimethylhexane
25	164	C_8H_{16} (isomer)
26	165-167	2,3,4-trimethylpentane
27	167-169	toluene
28	170	3-methylheptane
29	172-173	dimethylhexane isomer
30	174-176	n-octane
31	176-178	hexamethylcyclotrisiloxane (BKG)
32	178-179	tetrachloroethylene

(continued)

Table 58 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
32A	180	C_9H_{20} (isomer)
33	183	C_9H_{20} (isomer)
34	185	C_9H_{18} (isomer)
35	187-188	ethyl benzene and C_9H_{20} (isomer)
36	188-190	p-xylene
36A	191	C_9H_{18} (isomer)
36B	191	1-nonene
37	193	styrene
38	194-196	n-nonane and o-xylene
39	198	$C_{10}H_{20}$ (isomer)
40	200	isopropylbenzene
41	201	$C_{10}H_{22}$ (isomer)
41A	202	$C_{10}H_{20}$ (isomer)
42	203	$C_{10}H_{20}$ (isomer)
42A	204	$C_{10}H_{20}$ (isomer)
43	205-208	n-propylbenzene and $C_{10}H_{22}$ isomer and m-ethyltoluene
43A	208	$C_{10}H_{22}$ (isomer)
44	208-210	octamethylcyclotetrasiloxane (BKG) and $C_{10}H_{20}$ (isomer)
45	211	1-decene
46	212-214	n-decane and trimethyl benzene (isomer)
47	217	dichlorobenzene
48	219	$C_{11}H_{24}$ (isomer)
50	222	C_4-alkyl benzene (isomer)
51	224	C_4-alkyl benzene (isomer) and $C_{11}H_{22}$ (isomer)
53	229	$C_{10}H_{18}$ (isomer)
53A	229	C_4-alkyl benzene (isomer)
54	230	n-undecane

(continued)

Table 58 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
55	233	$C_{10}H_{20}$ (isomer)
55A	234	C_4-alkyl benzene (isomer)

[a] See Table 35 (S3) for sampling protocol.

Table 59. ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR IN HOBOKEN, NJ[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
2	73	CO_2
2A	79	ethylene oxide
3	79-82	CF_2Cl_2
3A	84	chloromethane
3B	86	isobutane
3C	89	1-butene
4	90	*n*-butane
4A	91	2-butene
5	92-94	acetaldehyde
7	102	isopentane
8	104	CCl_3F
9	106-107	C_5H_{10} (isomer) *and* furan
9A	108	*n*-pentane
9B	110	propanal *and* C_5H_{10} (isomer)
9C	111	ethanol
10	112	CH_2Cl_2
11	116-119	acetone
11A	120	isopropanol
12	122-123	2-methylpentane
12A	124	3-methylpentane
13	126-128	C_6F_6
14	128-130	*n*-hexane *and* 1-hexene
15	130-132	$CHCl_3$
16	132-135	C_7F_8
16A	135	methyl ethyl ketone
16B	136	1,2-dichloroethane
17	137	1,1,1-trichloroethane
17A	138	1,1-dichloropropane
18	143-144	benzene
19	144-145	CCl_4

(continued)

Table 59 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
19A	146	2-methylhexane
20	147	3-methylhexane
20A	148	C_7H_{14} (isomer)
21	149	C_8H_{16} (isomer)
22	150-152	trichloroethylene *and* 4,4-dimethyl-1-pentene *and* *n*-heptane
22A	153	C_8H_{16} (isomer)
23	155	methyl methacrylate *and* C_8H_{16} (isomer)
23A	158	C_7H_{14} (isomer)
24	159	C_8H_{18} (isomer)
25	162	C_8H_{16} (isomer)
26	164	C_8H_{18} (isomer)
27	165-168	toluene
28	168-169	2,4-dimethylhexane
29	171	C_8H_{16} (isomer)
30	173	*n*-octane
31	175	hexamethylcyclotrisiloxane (BKG)
32	177	tetrachloroethylene
32A	178	C_9H_{20} (isomer)
33	181	C_9H_{18} (isomer)
33A	182	C_9H_{18} (isomer)
33B	183	chlorobenzene
34	184	C_9H_{18} (isomer)
	185	C_9H_{20} (isomer)
35	187	ethylbenzene
36	188	*p*-xylene
36A	191	C_9H_{18} (isomer)
37	192	styrene
38	193	*n*-nonane *and* *o*-xylene

(continued)

Table 59 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
39	199	$C_{10}H_{22}$ (isomer)
40	200	$C_{10}H_{22}$ (isomer)
41	202	$C_{10}H_{20}$ (isomer)
	205	n-propyl benzene
42	206	benzaldehyde
	207	ethyl toluene
43	208	octamethylcyclotrisiloxane
45	212	n-decane
	213	1,2,4-trimethyl benzene
46	216	m-dichlorobenzene
47	218	1,2,3-trimethyl benzene
48	223	C_4-alkyl benzene
49	225	$C_{11}H_{20}$ (isomer)
50	228	$C_{11}H_{22}$ (isomer)
51	229	n-undecane
53	235	C_4-alkyl benzene

[a] See Table 35 (S4) for sampling protocol.

Table 60. ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR NEAR CELANESES CORPORATION, NEWARK, NEW JERSEY[a]

Chromatographic Peak No.[a]	Elution Temperature (°C)	Compound	μg/m^3
1	81	CF_2Cl_2	
2	83	methyl chloride	
2A	83	n-propane	
3	88	1-butene	
4	89	n-butane	
5	91	2-butene	
6	93	acetaldehyde	
7	97	ethyl chloride	
8	99	methyl bromide	
9	103	isopentane	
10	105	trichlorofluoromethane	
11	108	n-pentane	
12	110	propanal	
12A	110	furan	
12B	110	dimethyl ether	
13	113	acetone	
13A	113	methylene chloride	
14	116	C_6H_{14} isomer	
15	119	isopropanol	
16	123	C_7H_{14} isomer	
17	125	vinyl acetate	57
18	126	C_6H_{14} isomer	
19	129	[b]perfluorobenzene (S)	
20	130	n-hexane	
21	133	chloroform	37
22	136	[b]perfluorotoluene (S)	
23	139	2-butanone	200
24	141	1,1,1-trichloroethane	
25	144	benzene	300
25A	144	carbon tetrachloride	

(continued)

Table 60 (cont'd)

Chromatographic Peak No.[a]	Elution Temperature (°C)	Compound	μg/m^3
26	145	cyclohexane	
27	148	C_7H_{16} isomer	
28	149-166	methyl acrylate	4,545
29	168	n-butyl acetate	113
30	170	toluene	
31	172	C_8H_{16} isomer	
32	176	n-octane	
33	177	C_8H_{16} isomer	
34	178	tetrachloroethylene	
35	183	C_9H_{20} isomer	
36	185	chlorobenzene	
37	188	ethylbenzene	
38	190	p-xylene	
39	191	n-butyl acrylate	17
40	194	styrene	
41	195	o-xylene	
41A	195	n-nonane	
42	201	cumene	
43	202	$C_{10}H_{22}$ isomer	
44	204	$C_{10}H_{22}$ isomer	
45	205	n-propylbenzene	
46	207	m-ethyltoluene	
47	209	1,3,5-trimethylbenzene	
48	212	o-ethyltoluene	
49	214	1,2,4-trimethylbenzene	
49A	214	n-decane	
50	217	m-dichlorobenzene	
51	218	C_4-alkyl benzene	
52	220	1,2,3-trimethylbenzene	
53	221	$C_{11}H_{24}$ isomer	
54	224	C_4-alkyl benzene	

(continued)

Table 60 (cont'd)

Chromatographic Peak No.[a]	Elution Temperature (°C)	Compound	μg/m^3
55	225	C_4-alkyl benzene	
56	227	acetophenone	
57	229	C_4-alkyl benzene	
58	231	n-undecane	
59	233	$C_{11}H_{22}$ isomer	
60	235	$C_{12}H_{26}$ isomer	
61	238	C_4-alkyl benzene	
62	239	C_4-alkyl benzene	
63	240	C_5-alkyl benzene	
64	240	$C_{12}H_{26}$ isomer	
65	240	n-dodecane	
66	240	naphthalene	

[a] See Table 35 (S5) for sampling protocol.

Table 61. ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR IN STATEN ISLAND, NY[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	72	N_2, O_2
2	73	CO_2
3	80	CCl_2F_2 (Freon 12)
5	85	isobutane
6	92	acetaldehyde
7	97	$CHFCl_2$
8	98	CH_3NH_2 or $CHCH_2NH_2$ (tent.)
9	102	C_5H_{12} isomer
10	104	$CFCl_3$ (Freon II)
11	106	acetone
12	108	methyl n-propyl ether
13	111	CH_2Cl_2
14	112	2-methyoxyethyl acetate
15	115	dimethylbutane isomer
16	117	2-pentanol (tent.)
17	122	C_6H_{14} isomer
18	126	C_7H_{17} isomer
19	127	C_6F_6
20	129	C_7H_{14} isomer
21	131	$CHCl_3$
22	134	C_7F_8
23	137	n-butyl acetate
24	140	2-chloroethyl acetate
25	142	1,1,1-trichloroethane
26	144	benzene
27	145	CCl_4
28	146	2,3-dimethylpentane
29	147	C_6H_{12} isomer
30	149	C_7H_{16} isomer
31	151	trimethylpentane
32	153	C_7H_{16} isomer

(continued)

Table 61 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
33	154	isoamyl nitrile
33A	154	C_7H_{16} isomer
34	160	C_7H_{14} isomer
35	162	C_8H_{18} isomer
36	163	C_9H_{18} isomer
36A	163	C_9H_{18} isomer
37	165	$C_{10}H_{20}$ isomer
38	166	C_8H_{18} isomer
39	168	toluene
40	170	C_8H_{18} isomer
41	172	C_8H_{16} isomer
42	174	C_8H_{18} isomer
43	176	hexamethylcyclotrisiloxane (BKG)
44	178	tetrachloroethylene
45	186	chlorobenzene
46	188	ethylbenzene
47	190	p-xylene
48	193	styrene
49	195	o-xylene
50	196	$C_{10}H_{20}$ isomer
51	201	isopropylbenzene
51A	201	n-decyl chloride
54	208	acetophenone
55	212	trimethylbenzene
56	214	n-decane
56A	214	trimethylbenzene
56B	214	$C_{11}H_{20}$ isomer
58	220	$C_{10}H_{22}$ isomer
59	222	$C_{11}H_{20}$ isomer
60	223	$C_{11}H_{14}$ isomer
60A	223	$C_{11}H_{16}$ isomer
61	225	C_4-alkyl benzene

(continued)

Table 61 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
62	227	$C_{11}H_{20}$ isomer
62A	227	C_3-alkyl benzene
63	228	decamethyl cyclopentasiloxane
64	230	acetoxypropyltridecane (tent.)
65	231	C_4-alkyl benzene
65A	231	$C_{11}H_{20}$ isomer
66	238	$C_{11}H_{20}$ isomer
67	240	phenoxydiphenylether (tent.)

[a] See Table 35 (S6) for sampling protocol.

Table 62. ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR IN FORDS, NJ[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	60	N_2, O_2
2	62	CO_2
3	68	CF_2Cl_2
4	72	isobutane
5	77	chloropropane (tent.)
6	81	acetaldehyde
7	88	isopentane
8	90	CCl_3F
9	94	C_5H_{12}
10	98	CH_2Cl_2
11	100	dimethylbutane
12	101	diethyl ether
13	104	acetone
14	108	methylpentane
15	112	trimethylpentane
16	114	perfluorobenzene
17	116	C_7H_{14}
18	118	$CHCl_3$
19	119	diethyl sulfide
20	121	perfluorotoluene
21	126	1,1,1-trichloroethane
22	130	benzene
23	133	C_7H_{16} isomer
24	137	C_8H_{18} isomer
25	138	C_7H_{16} isomer
26	145	methylethylcyclopentane isomer
27	146	C_8H_{18} isomer
28	148	C_9H_{18} isomer
29	150	C_8H_{16} isomer
30	152	toluene
31	157	C_8H_{16} isomer
32	158	C_8H_{18} isomer

(continued)

Table 62 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
33	159	hexamethylcyclotrisiloxane (BKG)
34	161	tetrachloroethylene
35	165	C_9H_{20} isomer
36	169	chlorobenzene
37	172	ethylbenzene
38	173	xylene
39	178	cyclooctatetraene
40	179	xylene
41	179	C_9H_{20} isomer
42	180	C_9H_{20} isomer
43	182	ditolyl ether (?)
44	184	C_3-alkyl benzene
45	188	C_9H_{18} isomer
46	189	C_3-alkyl benzene
47	190	octamethylcyclotetrasiloxane (BKG)
48	191	benzaldehyde
49	193	C_4-alkyl benzene
50	197	C_3-alkyl benzene
51	200	C_9H_{18} isomer
52	202	dichlorobenzene
53	206	C_4-alkyl benzene
54	207	C_3-alkyl benzene
55	208	C_4-alkyl benzene
56	209	C_9H_{18} isomer
57	211	C_4-alkyl benzene
58	211	tolualdehyde
59	213	C_2-alkyl styrene (tent.)
60	214	$C_{11}H_{24}$ isomer
61	215	methyl benzoate (tent.)
62	217	C_4-alkyl benzene
63	218	dichlorotoluene (tent.)
64	220	_t_-butyl methyl ether (tent.)

(continued)

Table 62 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
65	224	C_4-alkyl benzene
66	225	trimethyl-1-methylethoxysilane
67	226	C_5-alkyl benzene
68	229	$C_{12}H_{26}$ isomer
69	232	naphthalene
70	233	methyl methyl benzoate
71	237	$C_{13}H_{28}$ isomer

[a] See Table 35 (S8) for sampling protocol.

Table 63. ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR IN BOUNDBROOK, NJ[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
1	63-4	difluordichloromethane
2	68	propane
3	74	1-butene
3A	75	*n*-butane
3B	76	2-butene
4	80	acetaldehyde
5	86	isopentane
6	87	chloroethane and trichlorofluormethane
6A	90	furan
6B	91	C_5H_{10} isomer
6C	92	*n*-pentane
7	96	dichloromethane
8	100	propanal
9	106	2-methylpentane
10	110	ter-butanol and 3-methylpentane
11	112	[c]hexafluorobenzene and *n*-hexane
12	115	chloroform
13	118	[c]perfluorotoluene
14	123	1,2-dichloroethane and 1,1,1-trichloroethane
15	127	benzene
15A	128	carbon tetrachloride
16	130	C_7H_{16} isomer and cyclohexane
17	132	isopropyl acetate
18	133	trichloroethylene and *n*-heptane
18A	134	ethyl acrylate
19	135	2,2-dimethyl-3-hexane
20	139	diisobutylene
21	141	dimethylcyclohexane isomer
22	144	C_7H_{16} isomer

(continued)

Table 63 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
23	145	methyl methacrylate
24	148	dimethylcyclohexane isomer
25	150	toluene
26	153	dimethylcyclohexane isomer
26A	155	C_8H_{14} isomer
27	156-7	_n_-octane
28	158-60	silane compound and tetrachloroethylene
28A	160	2-hexanone
29	165-8	chlorobenzene
30	169	ethyl benzene
30A	168	pyridine (tent.)
31	171	_p_-xylene
32	172	dibutyl ether
32A	173	C_9H_{18} isomer
33	175	styrene
34	176	_n_-nonane and _o_-xylene
34A	177	C_9H_{18} isomer
34B	178	C_9H_{16} isomer
35	181	isopropylbenzene
37	185	_n_-propylbenzene
38	187	_m_-ethyl toluene
39	188	phenol
40	189	benzaldehyde
41	191	silane compound
42	194	1,2,4-trimethylbenzene and _n_-decane
42A	197	aniline
43	198	_m_ or _p_-dichlorobenzene
43A	199	$C_{11}H_{24}$ isomer
44	200	1,2,3-trimethylbenzene and 2-methyl-2-pentenal (tent.)

(continued)

Table 63 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
44A	202	$C_{11}H_{20}$ isomer
45	203	o-dichlorobenzene
45A	204	sec-butylbenzene
46	205	m-diethylbenzene
46A	206	N-methylaniline
47	207	acetophenone
47A	208	fluoranisole (tent.)
48	211	nitrobenzene and n-undecane
48A	212	dimethylaniline isomer
49	214	C_4-alkyl benzene isomer
50	217	chloroaniline isomer
51	218	silane compound
52	222	$C_{12}H_{24}$ isomer
53	227	1,3,5-trichlorobenzene
54	229	naphthalene
56	233	1,2,4-trichlorobenzene
57	240	α-naphthylamine
58	240	β-methylnaphthalene
59	240	α-methylnaphthalene
60	240	2-ethyl quinoline

[a] See Table 35 (S9) for sampling protocol.

Table 64. ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR IN EL SEGUNDO, CA[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
3	42	CO_2
4	45	dichlorodifluormethane
6	48	propane
7	50	1-butene
8	51	_n_-butane
8A	51-3	SO_2
9	52	2-butene
12	55	acetaldehyde
14	60	isopentane
15	61	trichlorofluormethane
16	62	C_5H_{10} (isomer)
16A	63	furan
16B	63	C_5H_{10} (isomer)
17	64	_n_-pentane + propanal
18	65	dimethyl ether
18A	66-76	acetone
19	68	dichloromethane
19A	69	C_6H_{12} (isomer)
20	77	2-methylpentane
21	80	3-methylpentane
22	81	C_6H_{12} (isomer)
22A	82	C_6H_{14} (isomer)
23	83	hexafluorobenzene (?)
24	84	_n_-hexane
24A	85	C_6H_{12} (isomer)
25	86	chloroform
26	87	C_6H_{12} (isomer)
27	88	methyl ethyl ketone
28	89	C_6H_{12} (isomer)

(continued)

Table 64 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
29	90	perfluorotoluene (S)
30	92	methylcyclopentane
31	93	1,2-dichloroethane
32	94	1,1,1-trichloroethane
33	97	C_6H_{10} (isomer) and C_7H_{14} (isomer)
34	98	benzene and carbon tetrachloride
35	101	cyclohexane and 2-methylhexane
36	102	isopropyl acetate
37	103	3-methylhexane
39	105	dimethylcyclopentane isomer
40	106	dimethylcyclopentane isomer
41	107	trichloroethylene
41A	108	C_7H_{12} (isomer) and C_7H_{14} (isomer)
41B	108	3-methyl butanol (tent)
42	109	*n*-heptane
43	111	3-pentanone
43A	112	2-pentanone
44	113	2,4-dimethyl furan
44A	114	*n*-propyl acetate
45	116	methylcyclohexane
46	117	C_8H_{18} (isomer)
46A	117	C_8H_{16} (isomer)
46B	118	2,4-dimethylhexane
46C	118	C_7H_{14} (isomer)
47	119	4-methyl-2-pentanone
48	120	C_8H_{16} (isomer)
49	112	C_8H_{16} (isomer)
50	124-5	toluene (isomer)
51	125	C_8H_{18} (isomer)
51A	126	C_8H_{16} (isomer)

(continued)

Table 64 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
52	127	3-methylheptane
53	129	3-hexanone
53A	129	C_8H_{14} (isomer)
54	130	dimethylcyclohexane isomer + dimethylnitrosamine (tent.)
55	130-2	N,N-dimethyl formamide
56	132	C_8H_{16} (isomer)
57	134	n-octane
58	136	tetrachloroethylene
59	138	hexamethylcyclotrisiloxane(BKG)
60	140	C_9H_{20} (isomer)
61	141	C_8H_{16} (isomer)
62	142	C_9H_{20} (isomer)
62A	142	dimethylcyclohexane isomer
63	143	4-hydroxy-4-methyl-2-pentanone (tent) + chlorobenzene
64	144	C_9H_{18} (isomer)
65	147	ethylbenzene
65A	148	C_9H_{18} (isomer)
65B	148	C_9H_{20} (isomer)
66	149	p-xylene
66A	150	C_9H_{20} (isomer)
67	151	C_9H_{20} (isomer)
68	152	C_9H_{16} (isomer)
69	153	styrene
70	154	C_9H_{18} (isomer)
71	155	o-xylene
71A	156	C_9H_{18} (isomer)
72	157	n-nonane
72A	158	C_9H_{18} (isomer)

(continued)

Table 64 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
73	159	$C_{10}H_{20}$ (isomer)
74	160	methylethylcyclohexane isomer
75	161	$C_{10}H_{22}$ (isomer)
76	162	isopropylbenzene
77	162	$C_{10}H_{22}$ (isomer)
78	163	$C_{10}H_{20}$ (isomer)
78A	163	C_9H_{18} (isomer)
78B	164	C_9H_{16} (isomer)
79	164	$C_{10}H_{22}$ (isomer)
79A	165	propylcyclohexane + $C_{10}H_{20}$ isomer
80	165	$C_{10}H_{22}$ (isomer)
81	166	$C_{10}H_{20}$ (isomer)
82	168	benzaldehyde + n-propyl benzene
83	170	m-ethyl toluene + $C_{10}H_{22}$ (isomer)
84	170	$C_{10}H_{22}$ (isomer)
85	171	1,3,5-trimethylbenzene
86	172	$C_{10}H_{22}$ (isomer)
87	173	cyanobenzene or phenylisocyanide
88	174	o-ethyltoluene
89	175	$C_{10}H_{20}$ + $C_{10}H_{18}$ (isomer)
90	176	C_4-alkyl cyclohexane (isomer)
91	177	1,2,4-trimethylbenzene
92	178	n-decane
93	179	phenol
93A	179	$C_{10}H_{20}$ (isomer)
94	180	m-dichlorobenzene + $C_9H_{16}O$ (isomer + isobutylbenzene
94A	181	sec-butylbenzene
95	181	$C_{11}H_{24}$ (isomer)
95A	182	o-cymene

(continued)

Table 64 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
96	182	$C_{11}H_{24}$ (isomer)
97	183	1,2,3-trimethyl benzene
98	184	$C_{11}H_{24}$ (isomer)
98A	185	$C_{11}H_{22}$ (isomer)
99	186	o-dichlorobenzene
100	187	indan + C_4-alkyl cyclohexane (isomer)
100A	188	$C_{11}H_{22}$ (isomer)
101	188	C_4-alkyl benzene (isomer)
102	188	C_4-alkyl benzene (isomer)
103	189	C_4-alkyl benzene (isomer)
104	190	acetophenone
105	191	$C_{11}H_{22}$ (isomer)
106	192	$C_{11}H_{24}$ (isomer)
107	194	C_4-alkyl benzene (isomer)
108	195	C_4-alkyl benzene (isomer)
108A	196	$C_{11}H_{22}$ (isomer)
109	197	n-undecane
110	199	C_5-alkyl benzene (isomer)
110A	199	$C_{12}H_{26}$ + $C_{11}H_{22}$ (isomer)
111	200	$C_{11}H_{22}$ + C_4-alkyl benzene (isomers)
112	201	$C_{12}H_{26}$ (isomer)
113	202	1,2,4,5-tetramethylbenzene
114	203	$C_{12}H_{26}$ (isomer)
114A	204	C_5-alkyl benzene (isomer)
115	205	$C_{10}H_{16}O$ (isomer)
115A	205	$C_{12}H_{22}$ (isomer)
116	206	C_5-alkyl benzene (isomer)
116A	206	C_5-alkyl cyclohexane (isomer)
117	207	methyl indan (isomer)
117A	207	C_5-alkyl benzene (isomer)

(continued)

Table 64 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
118	208	$C_{12}H_{26}$ (isomer)
119	209	methyl indan (isomer)
119A	209	C_5-alkyl benzene (isomer)
120	210	$C_{12}H_{24}$ (isomer)
121	211	$C_{12}H_{26}$ (isomer)
122	212	C_5-alkyl benzene (isomer)
123	213	$C_{12}H_{22}$ (isomer)
123A	213	C_6-alkyl benzene (isomer)
124	214	$C_{12}H_{24}$ + dimethyl indan (isomers)
125	216	*n*-dodecane + naphtalene
125A	217	$C_{12}H_{24}$ (isomer)
125B	217	dimethyl indan (isomer)
126	218	$C_{13}H_{28}$ (isomer)
127	220	$C_{13}H_{28}$ (isomer)
128	221	$C_{13}H_{26}$ (isomer)
130	225	$C_{13}H_{26}$ (isomer)
131	226	$C_{13}H_{28}$ (isomer)
133	229	$C_{14}H_{30}$ (isomer)
133A	230	$C_{13}H_{26}$ (isomer)
134	231	$C_{13}H_{26}$ (isomer)
135	233	n-tridecane
136	235	$C_{14}H_{28}$ (isomer)
137	236	β-methylnaphthalene
138	239	α-methylnaphthalene
142	240	$C_{15}H_{32}$ (isomer)
143	240	n-tetradecane

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[a] See Table 36 (S1) for sampling protocol.

Table 65. ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR IN TORRANCE, CA[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
	41	CO_2
1	45	dichlorodifluormethane
2	47	chloromethane
3	48	_n_-propane
4	50	SO_2
5	50	1-butene
6	51	_n_-butane
7	52	2-butene
8	56	acetaldehyde
9	57-59	background
10	60	isopentane
11	62	trichlorofluormethane
11A	63	C_5H_{10} (isomer)
11B	63	furan + C_5H_{10} (isomer)
12	64	_n_-pentane
12A	65	C_5H_{10} (isomer)
13	66	propanal
13A	67	C_5H_{10} (isomer)
14	68	dichloromethane
14A	69-76	acetone
15A	77	C_6H_{12} (isomer)
15B	78	2-methylpentane
15C	80	C_6H_{12} (isomer)
16	82	3-methyl-pentane
17	83	$C_{16}H_{12}$ (isomer)
17A	84	$C_{16}H_{14}$ (isomer)
18	85	hexafluorobenzene (I)
19	85	_n_-hexane
20	86	chloroform
20A	87	C_6H_{12} (isomer)

(continued)

Table 65 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
21	88	methyl ethyl ketone
21A	90	C_6H_{12} (isomer)
22	92	perfluorotoluene (IS)
23	93	methylcyclopentane
24	94	1,2-dichloroethane
24A	95	C_7H_{16} (isomer)
25	96	1,1,1-trichloroethane
26	98	1,1-dichloropropene + C_6H_{10} + C_9H_{14} (isomers)
27	99	benzene
28	100	carbon tetrachloride
28A	101	cyclohexane
29	102	2-methyl hexane
30	103	C_7H_{16} (isomer)
31	104	3-methyl hexane
32	106	trimethyl pentane + C_7H_{14} (isomers)
33		unknown
34	108	trichloroethylene
35	110	n-heptane
36	112-114	2-pentanone + ethyl hydrazine
37	116	C_8H_{18} (isomer)
38	117	methyl cyclohexane
39	119	C_8H_{18} (isomer)
40	121	chloral
41	123	C_8H_{16} (isomer)
42	125	toluene
42A	126	C_8H_{18}
43	128	3-methylheptane
44	130	dimethylcyclohexane isomer
45	132	4-methyl-2-pentanone + 2,5-dimethyl-2,4-hexadiene

(continued)

Table 65 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
46	133	1,1,2-trichloropropene + C_8H_{16} (isomer)
47	134	n-octane
47A	135	C_8H_{16} (isomer)
48	136	tetrachloroethylene
49	138	silane compound
50	140	C_9H_{20} (isomer)
51	141	C_9H_{20} (isomer)
52	143-146	chlorobenzene
52A	147	trichloropropene (isomer)
53	148	ethyl benzene
53A	149	C_9H_{18} (isomer)
53B	149	C_9H_{20} (isomer)
54	150	p-xylene
55	151	dimethylheptane isomer
56	153	C_9H_{16} (isomer)
57	154	styrene
58	155	o-xylene
58A	156	C_9H_{18} (isomer)
59	157	n-nonane
59A	158	C_9H_{18} (isomer)
60	159	$C_{10}H_{20}$ (isomer)
60A	160	C_9H_{18} (isomer)
61	161	$C_{10}H_{22}$ isomer + 1,2,3,3-tetrachloropropene
62	162	isopropylbenzene + $C_{10}H_{22}$ isomer
62A	163	$C_{10}H_{22}$ (isomer)
63	163	tetrachloropropane (isomer) + 3,3,5-trimethylheptane
64	164	3-methylnonane
64A	165	$C_{10}H_{20}$ (isomer)

(continued)

Table 65 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
65	165	propylcyclohexane
66	166	$C_{10}H_{22}$ (isomer)
66A	167	$C_{10}H_{20}$ (isomer)
67	168	*n*-propylbenzene + benzaldehyde
68	169	*m*-ethyltoluene
69	170	$C_{10}H_{22}$ (isomer)
69A	170	1,3,5-trimethylbenzene
70	171	$C_{10}H_{22}$ (isomer)
71	172	$C_{10}H_{20}$ (isomer)
71A	173	cyanobenzene (tent)
72	174	*o*-ethyltoluene
73	175	octamethylcyclotetrasiloxane (BKG) + $C_{10}H_{20}$ + $C_{10}H_{18}$ isomers
74	176	$C_{10}H_{20}$ (isomer)
75	177	1,2,4-trimethylbenzene
76	178	*n*-decane
76A	179	$C_{10}H_{20}$ (isomer)
77	181	*m*-dichlorobenzene
78	182	C_4-alkyl benzene isomer
79	183	$C_{11}H_{24}$ (isomer)
80	184	1,2,3-trimethylbenzene
80A	184	$C_{11}H_{24}$ (isomer)
80B	185	$C_{11}H_{24}$ (isomer)
81	186	*o*-dichlorobenzene
81A	187	indan + C_4-alkyl cyclohexane isomer
82	188	*o*-cymene + $C_{11}H_{24}$ (isomer)
82A	188	sec-butylbenzene
82	189	C_4-alkyl benzene isomer
84	190	acetophenone
85	191	$C_{11}H_{24}$ (isomer)

(continued)

Table 65 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
86	192	$C_{11}H_{24}$ + C_4-alkyl benzene isomers
87	194	C_4-alkyl benzene + $C_{11}H_{22}$ isomers
88	195	methyl indan + $C_{12}H_{24}$ (isomers)
88A	196	$C_{11}H_{22}$ (isomer)
89	197	n-undecane
89A	198	$C_{11}H_{22}$ (isomer)
90	199	C_5-alkyl benzene + $C_{12}H_{26}$ (isomers)
91	200	C_4-alkyl benzene + $C_{12}H_{24}$ isomers
91A	201	$C_{12}H_{26}$ (isomer)
92	202	m-chlorobenzaldehyde
93	203	C_4-alkyl benzene (isomer)
93A	203	$C_{12}H_{26}$ (isomer)
93B	204	$C_{12}H_{24}$ + $C_{12}H_{22}$ (isomers)
94	205	C_5-alkyl benzene + $C_{11}H_{20}$ (isomers)
95	206	trichlorobenzene isomer
95A	206	C_5-alkyl cyclohexane (isomer)
96	207	methyl indan + $C_{12}H_{24}$ (isomers)
96A	207	C_{15}-alkyl-benzene (isomer)
97	207	$C_{12}H_{26}$ (isomer)
97A	208	$C_{12}H_{24}$ + C_5-alkyl benzene isomers
98	209	methyl indan (isomer)
98A	209	C_5-alkyl-benzene (isomer)
98B	210	$C_{12}H_{24}$ (isomer)
98C	210	C_4-alkyl benzene (isomer)
99	211	C_5-alkyl benzene (isomer)
99A	211	$C_{12}H_{24}$ (isomer)
100	212	$C_{13}H_{28}$ + C_5-alkyl benzene (isomers)

(continued)

Table 65 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
101	214	trichlorobenzene isomer
102	215	n-dodecane
103	216	naphthalene
103A	217	C_5-alkyl benzene (isomer)
103B	217	dimethyl indan (isomer)
104	218	$C_{13}H_{28}$ (isomer)
105	219	$C_{13}H_{26}$ (isomer)
106	221	trichlorobenzene (isomer)
106A	223	$C_{12}H_{26}$ (isomer)
107	225	$C_{13}H_{24}$ (isomer)
108	227	$C_{13}H_{28}$ (isomer)
109	228	$C_{14}H_{30}$ (isomer)
110	232	n-tridecane
111	234	$C_{14}H_{28}$ (isomer)
112	236	β-methylnaphthalene
113	238	α-methylnaphthalene
114	240	tetrachlorobenzene (isomer)
115	240	n-tetradecane
116	240	tetrachlorobenzene (isomer)

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[a] See Figure 31 and Table 35 (S2, Normandie Avenue) for sampling protocol.

Table 66. ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR FROM TORRANCE, CA[a]

Chromatographic Peak No.	Elution Temperature (°C)	Compound
3	43	CO_2
5	45	cyclopropane
6	46	difluorodichloromethane
8	48	propane
9	50	1-butene
10	50	n-butane
11	51	2-butene
12	54	acetaldehyde
13	56	C_4H_8 isomer
14	57	isopentane
14A	58	trichlorofluoromethane
14B	59	C_5H_{10} isomer
15	60	furan and C_5H_{10} isomer
15A	61	n-pentane
16	62	propanal and dimethyl ether
17	64	acetone and dichloromethane
17A	66	methyl silane
17B	68	C_6H_{12} isomer
18	74	2-methylpentane
19	77	3-methylpentane
20	78	C_6H_{12} isomer and C_6H_{14} isomer
21	80	hexafluorobenzene (Std.)
22	81	n-hexane
23	82	chloroform
23A	83	2-methylfuran
24	84	methyl ethyl ketone
25	87	perfluorotoluene (Std.)
26	88	methylcyclopentane
27	90	1,2-dichloroethane
28	91	1,1,1-trichloroethane
30	94	C_6H_{10} isomer and C_7H_{14} isomer
31	95	benzene

(continued)

Table 66 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
32	97	carbon tetrachloride
33	98	2-methylhexane
34	99	2,3-dimethylpentane
35	101	C_7H_{14} isomer
35A	102	3-methylhexane
36	103	C_7H_{14} isomer
37	104	1,2-dimethylcyclopentane
37A	104	C_7H_{14} isomer
38	105	trichloroethylene
38A	105	C_7H_{12} isomer
39	106	2-aminopentane (tent.)
40	107	n-heptane
41	109	2-pentanone and 2,4-dimethylfuran
42	113	2,2,4-trimethylpentane
43	114	methylcyclohexane
44	115	C_8H_{18} isomer
45	117	C_7H_{14} isomer
47	119	4-methyl-2-pentanone
48	121	C_8H_{16} isomer
49	124	toluene
50	125	C_8H_{18} isomer
51	126	2,4-dimethylhexane
51A	128	C_8H_{16} isomer
52	129	dimethylcyclohexane isomer
53	130	2-hexanone and C_8H_{14} isomer
54	131	methylethylcyclopentane isomer
55	133	n-octane
56	135	tetrachloroethylene
57	136	hexamethylcyclotrisiloxane
58	138	C_9H_{18} isomer

(continued)

Table 66 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
59	139	C_9H_{20} isomer
59A	140	C_9H_{18} isomer
60	141	C_9H_{20} isomer
61	142	C_9H_{20} isomer
62	143	dimethylcyclohexane isomer
63	144	chlorobenzene
64	145	1,2,3-trimethylcyclohexane
65	147	ethylbenzene
65A	148	C_9H_{16} isomer and C_9H_{18} isomer
66	148-50	p and m-xylene
67	151	C_9H_{20} isomer
68	152	N,N-dimethylformamide
68A	153	$C_7H_{14}O$ isomer
69	153	styrene
69A	154	C_9H_{18} isomer
70	155	p-xylene
70A	156	methylethylcyclohexane isomer
71	157	n-nonane
71A	158	C_9H_{18} isomer
72	159	$C_{10}H_{20}$ isomer
73	161	methylethylcyclohexane isomer
73A	161	$C_{10}H_{22}$ isomer
74	162	isopropylbenzene
75	163	$C_{10}H_{22}$ isomer
76	164	C_9H_{16} isomer
77	165	$C_{10}H_{22}$ isomer
78	166	propylcyclohexane
79	166	$C_{10}H_{20}$ isomer
80	167	benzaldehyde
81	169	n-propylbenzene

(continued)

Table 66 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
82	170	m-ethyltoluene
82A	171	$C_{10}H_{22}$ isomer
83	172	1,3,5-trimethylbenzene
84	173	$C_{10}H_{22}$ isomer
84A	173	cyanobenzene (tent.) and $C_{10}H_{20}$ isomer
84B	174	2-octanone (tent.)
85	175	o-ethyltoluene
86	176	$C_{10}H_{20}$ isomer
87	177	1-decene
88	178	1,2,4-trimethylbenzene
89	179	n-decane
90	180	phenol
91	181	isobutylbenzene and $C_{10}H_{20}$ isomer
91A	182	sec-butylbenzene
92	182	$C_{11}H_{22}$ isomer
92A	183	C_4-alkyl benzene isomer
93	183	$C_{11}H_{24}$ isomer
94	184	1,2,3-trimethylbenzene
95	185	$C_{11}H_{24}$ isomer
95A	186	$C_{11}H_{22}$ isomer
96	187	o-dichlorobenzene
97	187	indan
97A	188	C_4-alkylcyclohexane
97B	188	$C_{11}H_{22}$ isomer
98	189	p-propyltoluene
99	189.5	diethylbenzene isomer
100	190	n-butylbenzene
101	191	acetophenone
102	192	$C_{11}H_{22}$ isomer
103	193	o-propyltoluene

(continued)

Table 66 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
104	195	dimethylethylbenzene isomer
105	195	$C_{11}H_{22}$ isomer
106	196	dimethyl ethylbenzene isomer
107	197	methyl indan isomer
107A	198	$C_{11}H_{22}$ isomer
108	199	n-undecane
109	200	C_5-alkyl benzene isomer
110	201	C_4-alkyl benzene isomer + $C_{11}H_{22}$ isomer
111	202	$C_{12}H_{24}$ isomer
112	203	$C_{12}H_{26}$ isomer
113	204	1,2,4,5-tetramethylbenzene
114	205	$C_{12}H_{26}$ isomer
115	206	C_5-alkyl benzene isomer + $C_{11}H_{20}$ isomer
116	207	C_5-alkylcyclohexane isomer
117	208	methyl indan isomer or $C_{10}H_{12}$ + $C_{12}H_{24}$ isomer
118	209	$C_{12}H_{26}$ isomer
118A	210	$C_{11}H_{20}$ isomer
119	210	$C_{10}H_{12}$ isomer or methyl indan isomer
119A	211	tetramethylbenzene isomer + C_5-alkyl benzene isomer
120	212	C_5-alkyl benzene isomer
120A	213	$C_{12}H_{26}$ isomer
121	213	C_5-alkyl benzene isomer
122	214	C_4-alkyl benzene isomer
123	215	$C_{12}H_{24}$ isomer
124	216	1-dodecene + dimethylindan isomer
125	217	n-dodecane

(continued)

Table 66 (cont'd)

Chromatographic Peak No.	Elution Temperature (°C)	Compound
126	218	naphthalene
126A	218	C_5-alkyl benzene isomer
126B	219	dimethylindan isomer
127	220	$C_{13}H_{28}$ isomer
128	221	C_6-alkyl benzene isomer
129	223	$C_{13}H_{26}$ isomer
130	224	C_6-alkyl benzene isomer
131	225	benzothiazone (tent.)
132	227	$C_{13}H_{26}$ isomer
134	228	dimethylindan isomer
135	229	$C_{13}H_{26}$ isomer
136	230	$C_{14}H_{30}$ isomer
137	231	$C_{14}H_{28}$ isomer
138	232	$C_{13}H_{26}$ isomer
139	234	n-tridecane
140	236	trimethylindan isomer
	237	β-methylnaphthalene
141	237	$C_{14}H_{30}$ isomer
142	238	$C_{14}H_{30}$ isomer
143	240	α-methylnaphthalene
144	240	$C_{14}H_{30}$ isomer
145	240	$C_{14}H_{28}$ isomer
146	240	$C_{14}H_{30}$ isomer
148	240	$C_{15}H_{32}$ isomer
150	240	n-tetradecane
152	240	dimethylnaphthalene isomer + biphenyl
153	240	dimethylnaphthalene isomer

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[a] See Figure 31 and Table 35 (S2, Van Ness Blvd.) for sampling protocol.